I U C L I D

Data Set

Existing Chemical	:	ID: 68526-84-1
CAS No.	:	68526-84-1
EINECS Name	:	Alcohols, C8-10-iso-, C9-rich
EC No.	:	271-233-5
TSCA Name	:	Alcohols, C8-10-iso-, C9-rich
IUPAC Name	:	Alcohols C8-C10, Iso-, C9 rich

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.09.2004

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.09.2004
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	06.04.2006
Revision date	:	
Date of last update	:	06.04.2006
Number of pages	:	39
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C9H20O
Molecular weight : 144.26
Petrol class :

Flag : Critical study for SIDS endpoint
11.01.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 85566-14-9
IUPAC Name: Alcohols, C7-11-branched and linear
R Length (C number): C7 to C11
Structure of R: Linear
Category Member: No (analogue substance used for supporting information)

CAS RN: 68526-84-1
IUPAC Name: Alcohols C8-C10-iso, C9 rich
R Length (C number): C7
Structure of R: Branched, primarily methyl branched (isomeric structures)
Category Member: Yes

06.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Exxal(r) 9

12.03.2004

Isononanol

09.03.2004

Isononyl alcohol

09.03.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	68526-84-1
EC-No	:	271-233-5
EINECS-Name	:	Alcohols, C8-10-iso-, C9-rich
Molecular formula	:	C9H20O
Value	:	= 99.6 % w/w

Remark : Commercial product typically consists of dimethyl-1-heptanols and methyl-1-octanols.

06.01.2005

1.4 ADDITIVES

Purity type	:	typical for marketed substance
CAS-No	:	
EC-No	:	
EINECS-Name	:	
Molecular formula	:	
Value	:	
Function of additive	:	
Remark	:	No additives present

11.10.2005

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis
Remark	:	Primarily used as a chemical intermediate in the production of esters: phthalates, acetates, and adipates. Also frequently used in the paint industry.

06.01.2005

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -54 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: ASTM D97
Year	:	
GLP	:	no
Test substance	:	
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (1) (16)

2.2 BOILING POINT

Value	:	= 202 - 219 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078/01
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (16)

2.3 DENSITY

Type	:	density
Value	:	.832 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	1998
GLP	:	no data
Test substance	:	
Method	:	The density was measured by taking the weight of 10 mls of the test substance at 20 deg C.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(1) valid without restriction

06.04.2006 (11)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .054 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	no data
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (20)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 3.8 - 4.3 at 30 °C
pH value	:	
Method	:	OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1998
GLP	:	yes
Test substance	:	
Remark	:	Test Type: N-Octanol/Water Partition Coefficient (HPLC method)
Result	:	The test substance eluted as several groups. The three major components C8, C9, C10 alcohols had Log Pow values of 3.8, 4.2, and 4.3 respectively. The retention time for the 3 major components were 6.91, 8.42, and 8.96 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Test condition	:	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.

Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (13)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 90.4 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	1998
GLP	:	no data
Test substance	:	

Method	:	Water solubility calculated using WSKOWWIN ver 1.36 based on Kow correlation method of Meylan and Howard.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (5)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 90 °C
Type	:	closed cup
Method	:	other: PMCC ASTM D93
Year	:	
GLP	:	no data
Test substance	:	

Test substance	:	Analogue substance: Isononyl alcohol (CAS 27458-94-2)
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.

06.04.2006 (16)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.935 at 25°C
Method	:	other: calculated
Year	:	
GLP	:	no data
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (17)

2.13 VISCOSITY

Value	:	ca. 17 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	
GLP	:	no data
Test substance	:	other TS: Isononyl alcohol (CAS 27458-94-2)
Remark	:	Value measured in cSt
Test substance	:	Analogue substance: Isononyl alcohol (CAS 27458-94-2)
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.

26.10.2005 (16)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (15)

INDIRECT PHOTOLYSIS

Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000139469 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance :

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
9.2	13.95 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C

Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich

Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance. This robust summary represents a "key study" for atmospheric half-life range based on constituent data.

Flag : Critical study for SIDS endpoint

06.04.2006 (21)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: Technical Discussion
Year :
GLP :
Test substance :

Remark : These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.

Result : Hydolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis.

Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press, Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.

Flag : Critical study for SIDS endpoint

20.03.2006 (14)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	other: air - water - soil - sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level III
Year	:	2003

Method :

The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 144.26 g/mol
Water solubility = 90.4 mg/L
Vapour pressure = 5.4 Pa
log Kow = 4.05
Melting point = -54 deg C

Degradation half-lives:

Air - 9.2 hrs
Water - 120 hrs
Soil - 720 hrs
Sediment - 7200 hrs

This model was run assuming 100% discharge to water.

Result :

Air - 0.8%
Water - 79.5%
Soil - 0.03%
Sediment - 19.7%

Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are

calculated and not measured.

Flag : Critical study for SIDS endpoint
26.10.2005 (19)

Type : fugacity model level I
Media : other: air - biota - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level I
Year : 2003

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 144.26 g/mol
Water solubility = 90.4 mg/L
Vapour pressure = 5.4 Pa
log Kow = 4.05
Melting point = -54 deg C

Remark : Results were calculated using measured value for log Kow
Result : Air - 19.9%
Water - 7.2%
Soil - 71.3%
Sediment - 1.6%
Suspended Sed - 0.04%
Biota - <0.01%
Test substance : CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
26.10.2005 (19)

Type : volatility
Media : water - air
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculation
Year : 2005

Method : Henry's Law Constants (HLC) are based on vapor pressure and water solubility values, and molecular weights. HLC values were calculated using equations found in Mackay, 2003.

Vapor pressure = 5.4 Pa
Water solubility = 90.4 mg/l
Molecular mass = 144.26 g/mol

Result	:	HLC (at 25 deg C) = 8.62 Pa-m3/mole
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of (2) because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

26.10.2005 (19)

3.3.2 DISTRIBUTION

Media	:	other: Koc
Method	:	other (calculation)
Year	:	2005
Method	:	The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980). PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems.
Result	:	Koc = 43.71 log Koc = 1.64
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured. The value was calculated based on chemical structure as modeled by EPIWIN.

26.10.2005 (18) (22)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	at °C
Concentration	:	
BCF	:	15
Elimination	:	
Method	:	OECD Guide-line 305
Year	:	1998
GLP	:	yes
Test substance	:	
Remark	:	Duration: 16 days uptake, 10 days depuration The duration of the uptake phase was shorter than the guideline recommended duration of 28 days. The duration of the uptake phase was determined based on the concentration of the test substance reaching a steady state in the tissue of the fish. Samples of the fish were analyzed at

regular intervals. To determine the concentration of the test substance in the fish tissue, under steady-state conditions, one-tail T-tests for the comparison of the means at the sampling times were performed.
No difference in mortality or growth was observed between the treatments and the control after 16 days of exposure, or at the end of the study (26 days).

Result : Calculated Bioconcentration Factor (BCF):
0.75 mg/L = 14.8
0.15 mg/L = 15.5
Mean BCF for the study = 15.2

Test condition : A 100 mg/L stock solution was prepared by adding the appropriate amount of the test substance to 18 liters of dilution water. The stock solution was mixed for 24 hours prior to its use in the test. It was then pumped from the mixing vessel via a glass tube, silicon tubing and varistaltic pump and delivered to the test chambers via a 2 liter proportional diluter. Two concentrations were prepared for the test, 0.75 mg/L and 0.15 mg/L. A dilution water control was also prepared. A new stock solution was prepared in this manner every 4 days and mixed for 24 hours prior to use in the test.
One test chamber was prepared for each treatment and the control. At the start of the test each test chamber contained 45 fish. Fish were observed daily for mortality and/or abnormal behavior or appearance. Water and fish samples were removed periodically during both the uptake and depuration phases of the study. Samples were analyzed by gas chromatography.

Mean measured concentrations of the test substance in water :
0.75 mg/L = 0.91 mg/L (s.d.= 0.15)
0.15 mg/L = 0.16 mg/L (s.d.= 0.02)

The test substance was not detected in the control during the study or in either treatment during the depuration phase.
Mean measured concentrations of the test substance in fish tissue:
0.75 mg/L = 13.8mg/kg
0.15 mg/L = 2.5 mg/kg

Fish samples were also removed at the beginning and end of the uptake phase and analyzed for lipid content. The mean percent lipid content was 3.53%.

Test temperature was 14.6 Deg C., Lighting was 16 hours light : 8 hours dark with 438 to 612 Lux during full daylight periods.

Dissolved Oxygen ranged from 8.7 to 9.3 mg/L. The pH was ranged from 7.1 to 7.3 during the study. Fish were fed at a rate of 2% of their bodyweight per day during the study.

Fish Mean Weight was approximately = 0.367g at the start of the test. Test Loading = 0.47 g of fish/L.

Test substance : Read across from: Alcohols, C9-11-iso-, C10-rich (CAS. 68526-85-2)

Conclusion : The test substance is expected to have a low potential to bioaccumulate based on read across from the C10 alcohol. Value based on wet weight data.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.04.2006 (12)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 10.1 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1995
GLP	:	yes
Test substance	:	

Method : Bionomial Method

Result : LC50 = 10.1mg/L (CI 7.3 to 14.1), based upon measured concentrations of mean of old and new samples.

Analytical method used was GC-FID

LL50 = 11.2 mg/L (CI 7.5 to 16.6), based upon nominal loading levels.

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
0.7 mg/L	1.7 mg/L	0
1.5 mg/L	1.9 mg/L	0
3.3 mg/L	3.9 mg/L	0
7.5 mg/L	7.3 mg/L	0
16.6 mg/L	14.1 mg/L	100

Dissolved oxygen levels dropped below 60% of saturation in some of the treatments on Days 1 through 4 of the test. Since no mortality occurred in these treatments, the deviations are not believed to have affected the outcome of the study.

Test condition : Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.

Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 572 to 573 Lux during full daylight periods.
Dissolved Oxygen at initiation ranged from 8.4 to 9.0 mg/L and from 4.8 to 6.3 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.8 to 8.5 during the study. Fish were not fed during the study.

Fish Mean Wt.= 0.361g. Mean Total length = 3.8cm, Test Loading = 0.40 g of fish/L.

Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Test substance is considered to have moderate acute toxicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (11)

Type :

Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 7.6 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C9 alcohol with a Kow of 3.22.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected to have an acute 96-hour LC50 of 7.6 mg/L and a Chronic Value of 1.2 mg/L
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 4.9 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	1996
GLP	:	yes
Test substance	:	

Method	:	Probit procedure of SAS (Finney, 1971)
Remark	:	Test Type: Daphnid Acute Toxicity Test
Result	:	48-hour EC50 = 4.9 mg/L (CI 4.5 - 5.4), based upon measured concentrations of mean of old and new samples.

Analytical method used was Total Organic Carbon (TOC).

Nominal Conc.	Measured Conc.	% Immobilization @ 24 hr.
Control	0	0
1.56 mg/L	0.80 mg/L	0
3.12 mg/L	1.82 mg/L	0
6.25 mg/L	3.05 mg/L	0
12.5 mg/L	4.39 mg/L	40

25.0 mg/L 6.14 mg/L 85

Test condition : Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added to 2.0L of dilution water in a 2L glass aspirator bottle. The solutions were mixed for 25 hours at a vortex of </= 20% of the total depth. The test solutions were removed through the outlet at the bottom of each mixing vessel into four replicates of 140 mL in 125 mL glass erlenmeyer flasks (no headspace). Five daphnids were added to each test replicate and the replicates sealed. The test was performed under static conditions with no aeration.

Test temperature was 21.4 Deg C., Lighting was 16 hours light : 8 hours dark with 638 to 639 Lux during full daylight periods. Dissolved oxygen ranged from 7.3 to 8.2 mg/L during the study. The pH was ranged from 7.7 to 8.4 during the study.
Organisms were supplied by in-house cultures. Age = <24 hours old, from 13 and 16-day old parents.

Test substance : CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion : Test substance is considered to have moderate acute toxicity.
Reliability : (1) valid without restriction
Code 1, Reliable without Restrictions
Flag : Critical study for SIDS endpoint
06.04.2006 (10)

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 8.9 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C9 alcohol with a Kow of 3.22.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion : Based on the calculated Kow value, the C9 alcohol is expected to have an acute 48-hour EC50 of 8.9 mg/L and a Chronic Value of 0.8 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
06.04.2006 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: Pseudokirchneriella subcapitata

Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 6 calculated
ChV	:	= 1.207 calculated
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: ECOSAR Computer Model
Year	:	1999
GLP	:	no
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.22.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected to have an acute 96-hour EC50 of 6.0 mg/L and a Chronic Value of 1.207 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

Species	:	other algae: green alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.22. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected to have an acute 96-hour EC50 of 6.0 mg/L and a Chronic Value of 1.2 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= 1.196 calculated
Method	:	other: calculated
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.22.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected to have a 30-day Chronic Value of 1.196 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia sp. (Crustacea)
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= .778 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.22.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected yo have a 16-day EC50 of 0.778 mg/L.
Reliability	:	(2) valid with restrictions

The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
06.04.2006 (3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: Earthworm
Endpoint	:	
Exposure period	:	16 day(s)
Unit	:	mg/kg soil dw
LC50	:	= 373.58 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.22.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected yo have a 16-day EC50 of 373.58 mg/kg soil.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2979 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: None
Doses	:	34.6, 120, 417, 1450, 5000, or 10,000 mg/kg bw
Method	:	other: NA
Year	:	1968
GLP	:	no
Test substance	:	other TS
Remark	:	No deaths occurred in the 34.6, 120, 417, and 1450 mg/kg groups throughout the study. Two of the five animals in the 5000 mg/kg group died within 24 hours and all of the animals in the 10,000 mg/kg group died within 24 hours. Depression, labored respiration and evidence of excessive urination and/or diarrhea were observed at the 5,000 and 10,000 mg/kg dose levels. These signs of toxicity were observed within one hour of administration. At necropsy, abscessed lungs, dark red lungs and a dark zone between the renal cortex and medulla were observed in animals from the 5,000 and 10,000 mg/kg dose levels. Route of administration: Gastric Intubation Frequency of Treatment: Single Exposure Dose/Concentration Levels: 34.6, 120, 417, 1450, 5000 or 10,000 mg/kg Control group and Treatment: None
Result	:	LD50 = 2979 mg/kg
Test condition	:	After a three to four hour fasting period, groups of 5 rats (approximately 252-295 grams) received the undiluted test material at doses of 34.6, 120, 417, 1450, 5000 or 10,000 mg/kg body weight. Observations were recorded immediately after dosing; at one, four and 24 hours; and once daily for a total of 14 days.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Conclusion	:	Under conditions of this study, Alcohols, C8-10 iso, C9 rich have a low order of acute oral toxicity in rats.
Reliability	:	(2) valid with restrictions Pre-GLP. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

03.02.2005 (8) (27)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 3630 ppm
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	10
Vehicle	:	other: none
Doses	:	3630 ppm
Exposure time	:	6 hour(s)
Method	:	other

Year	:	1968
GLP	:	no
Test substance	:	other TS: isononyl alcohol (CAS No. 68526-84-1)
Remark	:	There were no deaths during the exposure, but 2/10 rats died during the first 14 hours post exposure. Systemic effects related to central nervous system depression were seen and these included inactivity, shallow, or labored respiration and prostration. Local irritation effects were seen, but quickly returned to normal at the termination of exposure.
Result	:	LC50 > 3630 ppm (approximately 21.7 mg/l)
Test condition	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 14-day post-exposure observation period. Feed and water were freely available during the post-exposure holding period. The experimental atmosphere was generated by metering a measured amount of the test substance with a Harvard infusion pump into a positive pressure spray nozzle situated within the chamber. Chamber concentrations were not determined. The nominal concentration was determined by the ratio of the weight of the test substance aerosolized to the total chamber airflow per unit time. After exposure, the animals were removed from the chamber and group housed by species.
Conclusion	:	Under the conditions of this study, isononyl alcohol has a low order of acute inhalation toxicity in rats.
Reliability	:	(2) valid with restrictions Pre-GLP, vapor concentration not analyzed. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

16.03.2006 (7) (27)

Type	:	LC50
Value	:	> 3630 ppm
Species	:	mouse
Strain	:	Swiss
Sex	:	male
Number of animals	:	10
Vehicle	:	other: none
Doses	:	3630 ppm
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1968
GLP	:	no
Test substance	:	other TS: isononyl alcohol (CAS No. 68526-84-1)
Remark	:	There were no deaths during the exposure, but 1/10 mice died during the first 14 hours post exposure. Systemic effects related to central nervous system depression were seen and these included inactivity, shallow, or labored respiration and prostration. Local irritation effects were seen, but quickly returned to normal at the termination of exposure.
Result	:	LC50 > 3630 ppm (approximately 21.7 mg/l)
Test condition	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 14-day post-exposure observation period. Feed and water were freely available during the post-exposure holding period. The experimental atmosphere was generated by metering a measured amount of the test substance with a Harvard infusion pump into a positive pressure spray nozzle situated within the chamber. Chamber concentrations were not determined. The nominal concentration was determined by the ratio of the weight of the test substance aerosolized to the total chamber airflow per unit time. After exposure, the animals were removed from the chamber and group housed by species.
Conclusion	:	Under the conditions of this study, isononyl alcohol has a low order of acute inhalation toxicity in mice.
Reliability	:	(2) valid with restrictions

Pre-GLP, vapor concentration not analyzed. From peer reviewed literature.

Flag : Critical study for SIDS endpoint

16.03.2006 (7) (27)

Type	:	LC50
Value	:	> 3630 ppm
Species	:	guinea pig
Strain	:	Hartley
Sex	:	male
Number of animals	:	10
Vehicle	:	other: none
Doses	:	3630 ppm
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1968
GLP	:	no
Test substance	:	other TS: isononyl alcohol (CAS No. 68526-84-1)
Remark	:	There were no deaths during the exposure. No guinea pigs died during the study. Systemic effects related to central nervous system depression were seen and these included inactivity, shallow, or labored respiration and prostration. Local irritation effects were seen, but quickly returned to normal at the termination of exposure.
Result	:	LC50 > 3630 ppm (approximately 21.7 mg/l)
Test condition	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 14-day post-exposure observation period. Feed and water were freely available during the post-exposure holding period. The experimental atmosphere was generated by metering a measured amount of the test substance with a Harvard infusion pump into a positive pressure spray nozzle situated within the chamber. Chamber concentrations were not determined. The nominal concentration was determined by the ratio of the weight of the test substance aerosolized to the total chamber airflow per unit time. After exposure, the animals were removed from the chamber and group housed by species.
Conclusion	:	Under the conditions of this study, isononyl alcohol has a low order of acute inhalation toxicity guinea pigs.
Reliability	:	(2) valid with restrictions Pre-GLP, vapor concentration not analyzed. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

16.03.2006 (7) (27)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: none
Doses	:	50, 200, 794, and 3160 mg/kg bw
Method	:	other
Year	:	1968
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	No deaths were observed at any timepoint in this study. No evidence of systemic toxicity was observed. Dose-related moderate to severe skin irritation was produced. For all of the doses tested, no compound-related

alterations were observed at necropsy.
Route of administration: Dermal
Frequency of Treatment: Single Exposure
Dose/Concentration Levels: 50, 200, 794 and 3160 mg/kg

Result : LD50 > 3160 mg/kg of body weight.
Test condition : A single application of the test material was made to four groups of four rabbits (2.0 to 2.8 kg) at doses of 50, 200, 794 and 3160 mg/kg. The material was applied to abraded abdominal skin under occlusive dressing. Observations were recorded immediately following application; at one, four and 24 hours; and once daily thereafter for a total of 14 days.
Conclusion : Under the conditions of this study, Alcohols, C8-10 iso, C9 rich has a low order of acute dermal toxicity in rats.
Reliability : (2) valid with restrictions
Pre-GLP. From peer reviewed literature.
Flag : Critical study for SIDS endpoint
03.02.2005 (8) (27)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 16
Vehicle : other: none
PDII :
Result : moderately irritating
Classification :
Method : other: similar to OECD TG 404
Year : 1968
GLP : no
Test substance : other TS: (CAS No. 68526-84-1)

Remark : A single 24-hour application of Alcohols, C8-10 iso-, C9 rich to intact rabbit skin produced marked irritation. Skin irritation consisted of slight to severe erythema, slight to moderate edema and atonia and slight to severe desquamation persisted to termination on day 14.
Result : Markedly irritating.
Test condition : Alcohols, C8-10 iso-, C9 rich was applied to the clipped, abdominal skin of 4 groups of 4 rabbits. Each application consisted of 0.05, 0.2, 0.794, or 3.16 g/kg test material under an occlusive dressing which was left in place for 24 hours. Measurements were made at 1 hour and at 24, 48 and 72 hours after dressing removal and continued daily for 14 days.
Conclusion : Under the conditions of the study, Alcohols, C8-10 iso-, C9 rich produced marked irritation to rabbit skin.
Reliability : (2) valid with restrictions
Pre-GLP.
Flag : Critical study for SIDS endpoint
04.01.2005 (9) (27)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : .1 undiluted
Dose :

Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	none
Result	:	moderately irritating
Classification	:	
Method	:	other: similar to OECD TG 405
Year	:	1968
GLP	:	no
Test substance	:	other TS
Remark	:	Mean scores at 24, 48, and 72 hours were 3, 2.83, 2 for conjunctival redness, 1.33, 0.17, 0 for chemosis, 1.67, 1.67, 0.67 for discharge, 1, 0.83, 0.17 for iridial irritation, and 1.17, 1 and 0.83 for corneal opacity, respectively. Maximum Group Draize score = 33 (out of 110) The test substance produced marked irritation in the eyes of rabbits which generally cleared by 10 days.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The untreated eye served as the control. The eyes of each animal were examined 1, 4, 24, 48, and 72 hours, and 4, 7 and 10 days after administration. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale. Body weights were determined at study initiation and termination.
Test substance	:	CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability	:	(2) valid with restrictions Pre-GLP. From peer reviewed literature.

04.01.2005 (6) (27)

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	none
Result	:	moderately irritating
Classification	:	
Method	:	other: OECD TG 405; EEC 84/449, section B.5
Year	:	1993
GLP	:	yes
Test substance	:	other TS
Remark	:	Mean scores at 24, 48, and 72 hours were 1.8, 1.3, 1.2 for conjunctival redness, 1.3, 1.2, 0.67 for chemosis, 1.3, 0.5, 0.17 for discharge, 0.83, 0.67, 0.33 for iridial irritation, and 0.83, 0.83 and 0.83 for corneal opacity, respectively. Maximum Group Draize score = 23.2 (out of 110) The test substance produced significant conjunctival irritation in the eyes of rabbits which generally cleared by 7 days.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water.

The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the right eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The untreated eye served as the control.

The eyes of each animal were examined 1, 24, 48, and 72 hours, and 7 days after administration. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.

Test substance : CAS No. 68526-84-1; Alcohols, C8-C10-iso, C9 rich
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

09.03.2004 (26)

5.3 SENSITIZATION

Type : other: Human Maximization (as described by Epstein and Kligman)
Species : human
Number of animals :
Vehicle : petrolatum
Result : not sensitizing
Classification : not sensitizing
Method : other: not specified
Year :
GLP : no data
Test substance : other TS

Remark : The test substance was prepared and administered as a 1% solution of 1-hexanol in petrolatum.
Test substance : Analog substance: 1-hexanol (CAS 111-27-3)
Reliability : (4) not assignable
This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.

11.10.2005 (24)

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat
Sex : male
Strain : Wistar
Route of admin. : other: Oral gavage
Exposure period : 14 days
Frequency of treatm. : once/day
Post exposure period :
Doses : 144 mg/kg bw
Control group : yes, concurrent vehicle
NOAEL : >= 144 mg/kg
Method : other
Year : 1983
GLP : no data
Test substance : other TS

Method : Mean values compared to controls by Student's t-test.
Remark : Isononanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Isononanol did not induce any changes in glycogen vacuolation or fat vacuolation. The levels of cholesterol and triglyceride were not

significantly different between animals treated with isononanol and vehicle controls. There was a slight induction of palmitoyl CoA oxidase activity. However, the activity of other peroxisome-associated enzymes was not affected and overall peroxisome number was not effected. No hyperlipidemia was observed.
Type of Study: 14-Day Repeated Dose
No. of animals/sex/dose: 5/treatment, 10/control; 1mmol/kg/day of isononanol (144 mg/kg/day)
Vehicle: Polyethylene glycol 300

Result : NOAEL >= 144 mg/kg/day

Test condition : After acclimation for 1 week, five animals received 1mmol/kg/day (144 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined.

Test substance : Isononanol

Conclusion : Under the conditions of this study, isononanol has a low order of sub-acute toxicity in male rats for the endpoints studied.

Reliability : (2) valid with restrictions
From peer reviewed literature. Screening study with limited examinations but scientifically valid and well documented.

16.03.2006 (25)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Cytogenetic assay
Species : rat
Sex :
Strain :
Route of admin. : gavage
Exposure period :
Doses : 2.26-12.8 mg/kg (1/5 LD50)
Result : negative
Method :
Year : 1987
GLP :
Test substance :

Method : Each 10 rats were investigated, 1 ml test article/rat was orally administered by gavage as a 40% suspension in water. Preparation of bone marrow 48 h after administration and microscopic analysis of 50 cells per animal.

Number of cells investigated was too few to correspond to scientific and regulatory requirements.

Original reference in Russian.

Result : 3% of cells with aberration were observed, control group 0% of cells with aberrations.

Test substance : Analogue substance: CAS No. 28473-21-4; nonanol

Reliability : (2) valid with restrictions
Documentation insufficient for complete assessment since reference is in a foreign language. However, reference is from a peer reviewed journal.

06.04.2006 (2)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	Gestation days 1-19
Frequency of treatm.	:	7 hrs/day
Duration of test	:	Animals were sacrificed on day 20 of gestation
Doses	:	150 mg/m3 (Saturated vapors)
Control group	:	other: 15 sham-exposed rats
NOAEL maternal tox.	:	= 150 mg/m³
Method	:	other
Year	:	1989
GLP	:	no data
Test substance	:	other TS
Method	:	MANOVA, ANOVA, Kruskal-Wallis test
Remark	:	No treatment-related effects were observed in dams. There were no statistically significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. There were no statistically significant differences between the mean number of corpora lutea and resorptions, the sex ratio, and the mean fetal weights between the control and treated groups. No. of animals/sex/dose: 15 dams/dose
Result	:	NOAEL = 150 mg/m3
Test condition	:	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.
Test substance	:	Analog substance: 1-Nonanol
Conclusion	:	Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Nonanol does not induce maternal or fetal toxicity.
Reliability	:	(2) valid with restrictions 2 - Reliable with restrictions - Similar to guideline study; only one exposure level.

11.10.2005 (23)

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	other: Oral gavage
Exposure period	:	Gestation days 6-15
Frequency of treatm.	:	daily
Duration of test	:	Animals sacrificed on gestation day 20
Doses	:	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Control group	:	yes
NOAEL maternal tox.	:	= 144 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1989
GLP	:	yes
Test substance	:	other TS
Method	:	Dunnett's test, Fisher's exact test
Remark	:	At the lowest dose level, no maternal toxicity was observed. There were an increased number of fetuses with hydroureter. However, the significance of this endpoint as an indicator of marginal developmental toxicity is questionable. At both the 144 and 720 mg/kg/day dose levels, there were no effects on the following parameters: uterine weight, conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, and viable fetuses. At the 720 mg/kg/day level, the following signs of maternal toxicity were observed - reduced food consumption, reduced body weight, unsteady gait, and reddish nasal discharge. Fetal effects included a slightly reduced mean fetal body weight and an increased number of fetuses with hydroureter. Signs of maternal toxicity at the 1440 mg/kg/day level included reduced rood consumption and mean body weight, severe clinical symptoms like abdominal or lateral position, and unsteady gait. In addition, 7 of the animals found dead by gestation day 11 and the remaining 3 were sacrificed in moribund condition by gestation day 10. At necropsy, all animals had light brown-gray discoloration of the liver and some had evidence of lung edema and petechiae in the lungs. Because of the death of all dams within the high dose group, no data were available to assess uterus weight, reproduction parameters, or fetal effects. No. of animals/sex/dose: 10/dose Vehicle: Aqueous emulsion in 0.005% Cremophor EL Control group and Treatment: Control Group 1: Doubly distilled water Control Group 2: Doubly distilled water with 0.005% Cremophor EL
Result	:	NOAEL = 144 mg/kg/day (Maternal and Fetal)
Test condition	:	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Test substance	:	Analog substance: Isononylalcohol 1 (CAS No. 68515-81-1)
Conclusion	:	When administered by oral gavage under the conditions of this study, Isononylalcohol 1 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononylalcohol 1 does not alter reproductive parameters at doses that are not maternally toxic.

Reliability	:	(2) valid with restrictions 2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
11.10.2005		(4)
Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	other: oral gavage
Exposure period	:	Gestation days 6-15
Frequency of treatm.	:	daily
Duration of test	:	Animals were sacrificed on gestation day 20
Doses	:	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Control group	:	yes
NOAEL maternal tox.	:	= 144 - mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1989
GLP	:	yes
Test substance	:	other TS
Method	:	Dunnett's test, Fisher's exact test
Remark	:	At the lowest dose level, no maternal or fetal toxicity was observed. In addition, there were no changes in reproductive parameters. At the 720 mg/kg/day level, signs of maternal toxicity included unsteady gait, piloerection, salivation, and reduced body weight gain and food consumption. There was also an increased frequency of fetuses with hydroureter at this level. At this level, there were no significant changes in reproductive parameters. Although there was an increased number of late resorptions, this number was within the range of biologic variation, was not dose-dependent, and was therefore considered incidental. At the highest dose level, dams exhibited marked decreases in weight gain and food consumption, and displayed severe clinical symptoms, including unsteady gait, apathy, and abdominal or lateral position. One animal was found dead on gestation day 9 and two other dams were sacrificed in moribund condition on gestation days 8 and 109. At necropsy, light brown-gray discoloration of the liver, lung edema, and petechiae in the lungs, heart, or bladder were observed. Fetuses from the high dose group had markedly reduced mean fetal body weight, increased frequency of hydroureter, and a higher frequency of fetuses with skeletal variations and retardations. At the highest dose, there were no changes in fertility parameters. No. of animals: 10/group Control Group and Treatment: Control Group 1: Doubly distilled water Control Group 2: Doubly distilled water with 0.005% Cremophor EL
Result	:	NOAEL = 144 mg/kg/day
Test condition	:	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Test substance	:	Analog substance: Isononylalcohol 2 (CAS No. 68515-81-1)
Conclusion	:	When administered by oral gavage under the conditions of this study,

Isononylalcohol 2 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononyl alcohol 2 does not alter fertility parameters at doses that are not maternally toxic.

Reliability : (2) valid with restrictions
2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.

11.10.2005 (4)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Remark : Low potential for reproductive toxicity. Adequate data exists for developmental and subchronic studies that show no effect on reproductive organs.

02.10.2003

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 28473-21-4
CAS No.	:	28473-21-4
EINECS Name	:	nonan-1-ol
EC No.	:	249-048-6
TSCA Name	:	Nonanol
Molecular Formula	:	C9H20O

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	30.09.2004

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	30.09.2004
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	06.04.2006
Revision date	:	
Date of last update	:	06.04.2006
Number of pages	:	29
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C9H20O
Molecular weight : 144.26
Petrol class :

Flag : Critical study for SIDS endpoint
05.04.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 143-08-8; 28473-21-4
IUPAC Name: Nonan-1-ol
R Length (C number): C9
Structure of R: Linear
Category Member: Yes

05.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Nonanol

30.09.2004

Nonyl alcohol

30.09.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	28473-21-4
EC-No	:	249-048-6
EINECS-Name	:	
Molecular formula	:	C9H20O
Value	:	> 98 % w/w

Remark : Commercial product typically consists of approximately 80% 3,5,5-trimethylhexanol.

05.04.2006

1.4 ADDITIVES

Purity type	:	typical for marketed substance
CAS-No	:	
EC-No	:	
EINECS-Name	:	
Molecular formula	:	
Value	:	
Function of additive	:	

Remark : No additives present.
05.04.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primarily used as a chemical intermediate in the production of esters, and in fragrances.

05.04.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -18.7 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no data
Test substance	:	
Method	:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Test substance	:	CAS No. 28473-21-4; nonan-1-ol
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (15)

2.2 BOILING POINT

Value	:	= 192 - 204 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 28473-21-4; nonan-1-ol
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (8)

2.3 DENSITY

Type	:	density
Value	:	= .832 g/cm³ at 20 °C
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 28473-21-4; nonan-1-ol
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (8)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .4 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no data
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 28473-21-4; nonan-1-ol
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (13)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 3.2 - 4.9 at 30 °C
pH value	:	
Method	:	OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1998
GLP	:	yes
Test substance	:	
Remark	:	Test Type: N-Octanol/Water Partition Coefficient (HPLC method)
Result	:	The test substance eluted as several groups. The five major components C6, C7, C8, C9, C10 alcohols had Log Pow values of 3.2, 3.7, 4.4, 4.5 and 4.9 respectively. The retention time for the 5 major components were 6.55, 8.68, 13.3, 13.8, and 19.0 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Test condition	:	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.

Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.

The pH of the evaluated solutions was the same as the reference solution it was evaluated against.

The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.

Test substance : CAS No. 28473-21-4; nonanol
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
05.04.2006 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 128 mg/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Slow stir
Year	:	1998
GLP	:	no data
Test substance	:	

Method : Slow-stir water solubility vessels consisted of glass aspirator bottles with capacities of 4 to 12 L. The spigot at the bottom of the vessel was fitted with short length of Tefzel tubing and a #13 glass stopper. The bottle was rinsed with a mixture of 1:1 methylene chloride : acetone followed by 2,2,4-trimethyl pentane. The bottle was then air dried in a laboratory fume hood and rinsed three times with dilution water.

A glass stir bar was added to the bottle and then the bottle was filled with the appropriate amount of water. The test substance was added to the bottle at a loading of 100 mg/L and the solution stirred quiescently with little or no visible vortex on a magnetic stir-plate.

Mixing was stopped one hour prior to sampling. Samples were removed through the outlet at the bottom of the vessel. To avoid losses and to prevent contamination, the samples were analyzed immediately by either GC-MSD or GC-FID. Samples were taken on Days 1, 3, 7, and 21.

Test substance : CAS No. 28473-21-4; nonanol
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
05.04.2006 (10)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 86.1 °C
Type	:	closed cup
Method	:	other: PMCC ASTM D93
Year	:	2003
GLP	:	
Test substance	:	
Test substance	:	CAS No. 28473-21-4; nonanol
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (8)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.5 at 25°C
Method	:	other: calculated
Year	:	2003
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Test substance	:	CAS No. 28473-21-4; nonanol
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.04.2006 (9) (18)

2.13 VISCOSITY

Value	:	= 18 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	
GLP	:	no data
Test substance	:	other TS
Remark	:	Value measured in cSt

Test substance	:	CAS No. 28473-21-4; nonanol
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (8)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (7)

Type :
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm^3
Rate constant : = .000000000000139553 cm^3/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP :
Test substance :

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
9.2	13.96 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition	:	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3
Test substance	:	CAS No. 28473-21-4; nonanol
Reliability	:	(2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance. This robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (14)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other: Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.
Result	:	Hydolysis as a Function of Molecular Structure Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis. Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982). References: Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press,

Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.

Flag : Critical study for SIDS endpoint

20.03.2006 (6)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 144.26 g/mol
Water solubility = 128 mg/L
Vapour pressure = 40.0 Pa
log Kow = 3.8
Melting point = -18.65 deg C

Degradation half-lives:

Air - 12.1 hrs
Water - 360 hrs
Soil - 720 hrs
Sediment - 7200 hrs

This model was run assuming 100% discharge to water.

Result : Air - 2.1%
Water - 86.0%
Soil - 0.05%

Sediment - 11.9%

Test substance : CAS No. 28473-21-4; nonanol
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.04.2006 (12)

Type : fugacity model level I
Media : other: air - biota - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level I
Year : 2003

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.
Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 144.26 g/mol
Water solubility = 128 mg/L
Vapour pressure = 40.0 Pa
log Kow = 3.8
Melting point = -18.65 deg C

Result : Soil - 57.5%
Air - 6.3%
Water - 35.3%
Sediment - 0.8%
Suspended Sed - 0.02%
Biota - <0.01%

Test substance : CAS No. 28473-21-4; nonanol
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.04.2006 (12)

3.3.2 DISTRIBUTION

Media : other: Koc
Method : other (calculation)
Year : 2003

Method : The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980).

PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases

in soil, or between water and sediment in aquatic ecosystems.

Result : Koc = 52.14
log Koc = 1.72

Test substance : CAS No. 28473-21-4; nonanol

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured. The value was calculated based on chemical structure as modeled by EPIWIN.

Flag : Critical study for SIDS endpoint

05.04.2006 (11) (16)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic

Inoculum : activated sludge, domestic

Contact time :

Degradation : = 83.7 (±) % after 28 day(s)

Result : readily biodegradable

Deg. product :

Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"

Year : 1998

GLP : yes

Test substance :

Remark : Test Type: Manometric Respirometry Test
Exposure Period: 28 days

Result : Test material was readily biodegradable. Half-life was reached by day 6. By day 28, 83.7% degradation of the test material was observed. 10% biodegradation was achieved by day 2.

By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	85.8, 83.7, 81.8	83.7
Na Benzoate	87.1, 85.4	86.2

* replicate data

Test condition : Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 53 mg/L. Sodium benzoate (positive control) concentration was 50.6mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : CAS No. 28473-21-4; nonanol
Conclusion : Test substance is considered readily biodegradable.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
05.04.2006 (5)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	other: calculated
Species	:	other: frfeshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 6.4 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.30. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 28473-21-4; nonanol
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected to have an acute 96-hour LC50 of 6.4 mg/L and a Chronic Value of 1.0 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 7.5 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.30.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 28473-21-4; nonanol

Conclusion : Based on the calculated Kow value, the C9 alcohol is expected to have an acute 48-hour EC50 of 7.5 mg/L and a Chronic Value of 0.7 mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

05.04.2006 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: green alga
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 5.1 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C9 alcohol with a Kow of 3.30.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 28473-21-4; nonanol

Conclusion : Based on the calculated Kow value, the C9 alcohol is expected to have an acute 96-hour EC50 of 5.1 mg/L and a Chronic Value of 1.1 mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

05.04.2006 (2)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= 1 calculated
Method	:	other: calculated
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.30.
Test substance	:	CAS No. 28473-21-4; nonanol
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected to have a 30-day Chronic Value of 1.0 mg/L
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (2)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia sp. (Crustacea)
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= .7 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.30.
Test substance	:	CAS No. 28473-21-4; nonanol
Conclusion	:	Based on the calculated Kow value, the C9 alcohol is expected yo have a 16-day EC50 of 0.7 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (2)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: Earthworm
Endpoint	:	mortality
Exposure period	:	14 day(s)
Unit	:	mg/kg soil dw
LC50	:	= 353 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C9 alcohol with a Kow of 3.30.
Test substance	:	CAS No. 28473-21-4; nonanol
Conclusion	:	Based on the calculated Kow value, the C7 alcohol is expected to have a 14-day EC50 of 353 mg/kg soil.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (2)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	
Strain	:	
Route of admin.	:	inhalation
Exposure period	:	2 months
Frequency of treatm.	:	2 h/d
Post exposure period	:	none
Doses	:	0.2; 0.6; 0.8 mg/l
Control group	:	no data specified
Method	:	
Year	:	1964
GLP	:	
Test substance	:	
Method	:	Rats were exposed to concentrations of 0.2; 0.6 and 0.8 mg/l (33, 99 and 136 ppm) for 2h/day for 2 months.
Result	:	Small amounts of deformed or degenerate glial elements diffusely scattered in the cerebral cortex and subcortex were observed.
Test substance	:	CAS No. 28473-21-4; nonanol
Reliability	:	(4) not assignable Secondary literature, documentation insufficient for assessment. Can be used to support weight of evidence.

06.04.2006 (3)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	
Strain	:	
Route of admin.	:	gavage
Exposure period	:	
Doses	:	2.26-12.8 mg/kg (1/5 LD50)
Result	:	negative
Method	:	
Year	:	1987
GLP	:	
Test substance	:	

Method : Each 10 rats were investigated, 1 ml test article/rat was orally administered by gavage as a 40% suspension in water. Preparation of bone marrow 48 h after administration and microscopic analysis of 50 cells per animal.

Number of cells investigated was too few to correspond to scientific and regulatory requirements.

Original reference in Russian.

Result : 3% of cells with aberration were observed, control group 0% of cells with aberrations.

Test substance : CAS No. 28473-21-4; nonanol

Reliability : (2) valid with restrictions
Documentation insufficient for complete assessment since reference is in a foreign language. However, reference is from a peer reviewed journal.

06.04.2006 (1)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	Gestation days 1-19
Frequency of treatm.	:	7 hrs/day
Duration of test	:	Animals were sacrificed on day 20 of gestation
Doses	:	150 mg/m3 (Saturated vapors)
Control group	:	other: 15 sham-exposed rats
NOAEL maternal tox.	:	= 150 mg/m³
NOAEL teratogen.	:	= 150 - mg/m³
Method	:	
Year	:	1987
GLP	:	
Test substance	:	

Method : MANOVA, ANOVA, Kruskal-Wallis test

Remark : No treatment-related effects were observed in dams. There were no statistically significant differences in maternal weight gain, feed

consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. There were no statistically significant differences between the mean number of corpora lutea and resorptions, the sex ratio, and the mean fetal weights between the control and treated groups.
No. of animals/sex/dose: 15 dams/dose

Test condition : Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.

Test substance : CAS No. 28473-21-4; nonanol

Conclusion : Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Nonanol does not induce maternal or fetal toxicity.

Reliability : (2) valid with restrictions
Similar to guideline study; only one exposure level.

Flag : Critical study for SIDS endpoint

06.04.2006 (17)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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(3) Egorov, YuL and Adrianov LA, Uch. Zap. Mosk. Nauchn. - Issled Inst. Gig. 9, 47, (1961), In: Chemical Abstracts, 61, 3601 (1964) und 60, 12576d (1964), In: Clayton GD and Clayton FE (eds), Patty's Industrial Hygiene and Toxicology, Third Revised Edition in Three Volumes, Volumes 2A, 2B and 2C, Toxicology, New York (1982)

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 68526-79-4
CAS No.	:	68526-79-4
EINECS Name	:	Hexanol, branched and linear
EC No.	:	271-227-2
TSCA Name	:	Hexanol, branched and linear
Molecular Formula	:	Unspecified

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	04.04.2006
Revision date	:	
Date of last update	:	04.04.2006
Number of pages	:	36
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C6H14O
Molecular weight : 102.18
Petrol class :

Flag : Critical study for SIDS endpoint
03.04.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 111-27-3
IUPAC Name: hexan-1-ol
R Length (C number): C6
Structure of R: Linear
Category Member: No (analogue substance used for supporting information)

CAS RN: 68526-79-4
IUPAC Name: Hexanol, branched and linear
R Length (C number): C6
Structure of R: Branched, primarily methyl branched (isomeric structures)
Category Member: Yes

04.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Exxal 6

17.09.2004

hexyl alcohol

17.09.2004

isohexanol

17.09.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	68526-79-4
EC-No	:	271-227-2
EINECS-Name	:	Hexanol, branched and linear
Molecular formula	:	C6H14O
Value	:	= 98 % w/w

Remark : Commercial product typically consists of three isomers with the following composition: 44% 1-hexanol, 53% methyl pentanols, and 3% 2-ethylbutanol.

03.04.2006

1.4 ADDITIVES

Purity type : typical for marketed substance
CAS-No :
EC-No :
EINECS-Name :
Molecular formula :
Value :
Function of additive :

Remark : No additives present.
03.04.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primarily used as a chemical intermediate in the production of esters: phthalates and acetates.

03.04.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -49.3 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no
Test substance	:	
Method	:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (20)

2.2 BOILING POINT

Value	:	= 152 - 163 °C at 1013 hPa
Decomposition	:	
Method	:	other: D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (11)

2.3 DENSITY

Type	:	density
Value	:	= .827 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (11)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 2.56 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain. Result supplied by the experimental database in EPIWIN.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (17)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 1.8 - 2 at °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	
Test substance	:	
Method	:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (19)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 10340 - 11950 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no data
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (20)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 60.5 °C
Type	:	closed cup
Method	:	other: TCC ASTM D56
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (11)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.50 at 25°C
Method	:	other: calculated
Year	:	
GLP	:	no data
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

03.04.2006 (14)

2.13 VISCOSITY

Value	:	= 6.8 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.

03.04.2006 (11)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (10)

Type :
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm^3
Rate constant : = .0000000000099923 cm^3/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year :
GLP :
Test substance : other TS

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
12.8	9.99 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition	:	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life for the test substance.
Flag	:	Critical study for SIDS endpoint

17.09.2004 (18)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other: Technical Discussion
Year	:	
GLP	:	
Test substance	:	

Remark : These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.

Result : Hydolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis.

Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982).

References:

Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press, Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.
Flag : Critical study for SIDS endpoint
20.03.2006 (9)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 102.18 g/mol
Water solubility = 11950 mg/L
Vapour pressure = 256 Pa
log Kow = 1.75
Melting point = -49 deg C

Degradation half-lives:

Air - 12.9 hrs
Water - 120 hrs
Soil - 720 hrs
Sediment - 7200 hrs

This model was run assuming 100% discharge to water.

Result : Air - 0.3%
Water - 99.4%
Soil - 0.02%
Sediment - 0.28%

Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (16)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	
Year	:	1997
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 102.18 g/mol Water solubility = 11950 mg/L Vapour pressure = 256 Pa log Kow = 1.75 Melting point = -49 deg C
Result	:	Air - 29.5% Water - 67.0 % Soil - 3.3% Sediment - 0.1% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (16)

3.3.2 DISTRIBUTION

Media	:	other: Koc
Method	:	other (calculation)
Year	:	2003
Method	:	The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980). PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases

in soil, or between water and sediment in aquatic ecosystems.

Result	:	Koc = 7.30 log Koc = 0.86
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured. The value was calculated based on chemical structure as modeled by EPIWIN.

03.04.2006 (15) (21)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 97.7 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: no data
Year	:	1980
GLP	:	no data
Test substance	:	

Method : Trimmed Spearman Karber Method

Result : 96 hour LC50 = 97.7 mg/L (95% CI 89.7 to 106) based upon measured values

Analytical method used was Gas-Liquid Chromatography.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
26.7	0
49.2	0
90.6	20
170.0	50
261.5	50

* 50 fish added at test initiation

Test condition : Treatment solutions were prepared by diluting a 3720mg/L stock solution. Nominal hexanol treatment levels were 41, 68, 113, 189, 315mg/L, which measured 26.7, 49.2, 90.6, 170.0, and 261.5mg/L, respectively. Control/dilution water was EPA Duluth laboratory water. Fifty fish were tested per treatment, divided into two replicates. Treatment volume = 6.3L. Test parameters were as follows: temperature=26.2 Deg C; dissolved oxygen = 6.2mg/L; pH = 7.6; fish age = 28 days old; fish mean wt = 0.117g; fish mean length = 19.7mm; fish loading = 0.464g/L/day. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.

Test substance : CAS No. 68526-79-4; Hexanol, branched and linear

Reliability : (1) valid without restriction

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Type	:	
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 130.3 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a

database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C6 alcohol with a Kow of 1.75.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-79-4; Hexanol, branched and linear

Conclusion : Based on the calculated Kow value, the C6 alcohol is expected to have an acute 96-hour LC50 of 130 mg/L and a Chronic Value of 16.1 mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.04.2006 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 137 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C6 alcohol with a Kow of 1.75.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-79-4; Hexanol, branched and linear

Conclusion : Based on the calculated Kow value, the C6 alcohol is expected to have an acute 48-hour EC50 of 137 mg/L and a Chronic Value of 6.3 mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

03.04.2006 (4)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: Pseudokirchneriella subcapitata

Endpoint	:	biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	= 5 measured/nominal
EC50	:	= 89 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	2003
GLP	:	yes
Test substance	:	

Remark : Statistical Procedure - Proc regression procedure of SAS, Anova procedure of SAS for NOEC

Result : 72 hour EC50b=89 mg/L (biomass)
72 hour EC50gr=159 mg/L (growth rate)

72 hour NOECb=5 mg/L (biomass)
72 hour NOECgr=35 mg/L (growth rate)

Nominal Conc. (mg/L)	Biomass - 72 hr (% Inhibition)	Mean Cell Conc. - 72 hr (cells/ml)
Control	n/a	9.3 x105
6	5.2	8.9 x105
14	13	7.8 x105
34	16	7.8 x105
82	48	4.3 x105
196	94	6.1 x104

n/a - Not applicable

Test condition : Individual test treatment solutions were prepared as Water Accommodated Fractions (WAFs). Test material was added to algal media in 2.0L aspirator bottles. The mixing vessels were sealed with Teflon-covered stoppers and mixed on magnetic stir plates with teflon coated stir bars for 23 hours at room temperature. After mixing the solutions were allowed to settle for one hour and the WAF was removed from the bottom of the mixing vessel via the port and used for testing. Test vessels were 125ml glass Erlenmeyer flasks with approximately 60 ml of treatment solution and inoculated with algae. Test vessels were sealed with foam stoppers. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1.0 x 104 cells/ml. All test replicates were placed on a shaker table at 109 oscillations per minute during the study. Biomass was calculated as the area under the growth curve.

Nominal loading levels were 6, 14, 34, 82, and 196 mg/L

Test temperature was 23.0 Deg. C. Lighting was continuous at 7400 to 8200 Lux. The pH was 7.3 to 7.4 at test initiation and ranged from 6.9 to 7.3 at test termination.

Test treatments were analyzed by GC-FID. Measured values on Day 0 were 5.0, 12.7, 34.7, 83.4 and 182 mg/L. The test material was not detected in the control.

Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Test substance is considered to have moderate acute toxicity to aquatic plants.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

03.04.2006 (8)

Species	:	other algae: green alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 84 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C6 alcohol with a Kow of 1.75. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Based on the calculated Kow value, the C6 alcohol is expected to have an acute 96-hour EC50 of 84 mg/L and a Chronic Value of 7.3 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

03.04.2006 (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= 16.1 calculated
Method	:	other: calculated
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C6 alcohol with a Kow of 1.75.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear

Conclusion	:	Based on the calculated Kow value, the C6 alcohol is expected to have a 30-day Chronic Value of 16.1 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (3)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia magna (Crustacea)
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= 6.3 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C6 alcohol with a Kow of 1.75.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Based on the calculated Kow value, the C6 alcohol is expected yo have a 16-day EC50 of 6.3 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: Earthworm
Endpoint	:	mortality
Exposure period	:	14 day(s)
Unit	:	mg/kg soil dw
LC50	:	= 750.5 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C6 alcohol with a Kow of 1.75.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Based on the calculated Kow value, the C6 alcohol is expected to have a 14-day EC50 of 750.5 mg/kg soil.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (3)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 3670 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: None
Doses	:	
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	None of the animals died in the 26, 82, 259, and 820 mg/kg dose groups. One of the animals in the 2591 mg/kg group died within 24 hours of dosing. All animals in the 8200 mg/kg group died within 4 hours following dose administration. Treatment resulted in depression (i.e. inactivity, depressed righting reflexes, ataxia) and labored respiration. These signs had an early onset and recovery was complete by the second day after dosing. Gross necropsy on the animals that died showed congested kidneys. Also, animals that died during the first hour after administration showed evidence of gastrointestinal irritation. Route of administration: Gastric Intubation Frequency of Treatment: Single exposure Dose/Concentration Levels: 26, 82, 259, 820, 2591, 8200 mg/kg Control group and Treatment: None
Result	:	LD50= 3670 mg/kg
Test condition	:	After a three to four hour fasting period, groups of 5 rats received the test material at dose levels of 26, 82, 259, 820, 2591, and 8200 mg/kg of body weight. The results were converted to weight units by means of the specific gravity. Observations for signs of toxicity were made immediately and at one and 24 hours after compound administration and daily for a period of 7days. Gross necropsy examinations were performed on all animals that died or were killed.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Under the conditions of this study, Hexanol, branched and linear has a low order of acute oral toxicity in rats.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

03.04.2006 (13)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 1060 ppm
Species	:	rat
Strain	:	Wistar
Sex	:	male
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)

Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	No deaths were seen during or after the exposure period. Thirty minutes after exposure, slow, deep respiration was observed. After 90 minutes of exposure, the rats exhibited gasping, labored respiration, lacrimation and nasal discharge. These signs persisted until the termination of exposure. Gross necropsy results indicate that the test material produced slight lung congestion in all animals. All other tissues and organs were unremarkable. Route of administration: Inhalation Frequency of Treatment: Single 6 hour exposure Dose/Concentration Levels: 1060 ppm Control group and Treatment: None
Result	:	LC50 > 1060 ppm for rats.
Test condition	:	Rats received a single, 6-hour exposure to the test material in air. Exposures were at atmospheres nearly saturated with vapors of the alcohol (1060 ppm). The exposure was conducted in a 500-liter stainless steel inhalation chamber equipped at the inlet with a device for generating a near-saturated vapor of the test material. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml. Of the test material. Air flow through each bubbler was 18 liters/minute, so the total flow through the chamber was 36 liters/min. Actual chamber concentration was not measured during the exposure. The theoretical chamber concentration was calculated to be 1060 ppm based upon the amount of test material that vaporized and the rate of air flow. During exposure, all animals were observed for gross signs of toxicity at 30-minute intervals. Gross necropsies were performed on animals 24 hours after exposure.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Under the conditions of this study, Hexanol, branched and linear has a low order of acute inhalation toxicity in rats.
Reliability	:	(2) valid with restrictions No analysis of exposure atmosphere.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (13)

Type	:	LC50
Value	:	> 1060 ppm
Species	:	mouse
Strain	:	Swiss
Sex	:	male
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	No deaths were seen during or after the exposure period. Thirty minutes after exposure, slow, deep respiration was observed. After 90 minutes of exposure, the mice exhibited gasping, labored respiration, lacrimation and nasal discharge. These signs persisted until the termination of exposure. Gross necropsy results indicate that the test material produced slight lung congestion in all animals. All other tissues and organs were unremarkable. Route of administration: Inhalation Frequency of Treatment: Single 6 hour exposure Dose/Concentration Levels: 1060 ppm Control group and Treatment: None

Result	:	LC50 > 1060 ppm for mice.
Test condition	:	Mice received a single, 6-hour exposure to the test material in air. Exposures were at atmospheres nearly saturated with vapors of the alcohol (1060 ppm). The exposure was conducted in a 500-liter stainless steel inhalation chamber equipped at the inlet with a device for generating a near-saturated vapor of the test material. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml. Of the test material. Air flow through each bubbler was 18 liters/minute, so the total flow through the chamber was 36 liters/min. Actual chamber concentration was not measured during the exposure. The theoretical chamber concentration was calculated to be 1060 ppm based upon the amount of test material that vaporized and the rate of air flow. During exposure, all animals were observed for gross signs of toxicity at 30-minute intervals. Gross necropsies were performed on animals 24 hours after exposure.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Under the conditions of this study, Hexanol, branched and linear has a low order of acute inhalation toxicity in mice.
Reliability	:	(2) valid with restrictions No analysis of exposure atmosphere.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (13)

Type	:	LC50
Value	:	> 1060 ppm
Species	:	guinea pig
Strain	:	other: English short hair
Sex	:	male
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	No deaths were seen during or after the exposure period. Thirty minutes after exposure, slow, deep respiration was observed. After 90 minutes of exposure, the guinea pigs exhibited gasping, labored respiration, lacrimation and nasal discharge. These signs persisted until the termination of exposure. Gross necropsy results indicate that the test material produced slight lung congestion in all animals. All other tissues and organs were unremarkable. Route of administration: Inhalation Frequency of Treatment: Single 6 hour exposure Dose/Concentration Levels: 1060 ppm Control group and Treatment: None
Result	:	LC50 > 1060 ppm for guinea pigs.
Test condition	:	Guinea pigs received a single, 6-hour exposure to the test material in air. Exposures were at atmospheres nearly saturated with vapors of the alcohol (1060 ppm). The exposure was conducted in a 500-liter stainless steel inhalation chamber equipped at the inlet with a device for generating a near-saturated vapor of the test material. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml. Of the test material. Air flow through each bubbler was 18 liters/minute, so the total flow through the chamber was 36 liters/min. Actual chamber concentration was not measured during the exposure. The theoretical chamber concentration was calculated to be 1060 ppm based upon the amount of test material that vaporized and the rate of air flow. During exposure, all animals were observed for gross signs of toxicity at 30-minute intervals. Gross necropsies were performed on animals 24 hours

after exposure.

Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Under the conditions of this study, Hexanol, branched and linear has a low order of acute inhalation toxicity in guinea pigs.
Reliability	:	(2) valid with restrictions No analysis of exposure atmosphere.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (13)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2600 mg/kg bw
Species	:	rabbit
Strain	:	other: Albino
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: None
Doses	:	
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Dermal Application Frequency of Treatment: Single exposure Dose/Concentration Levels: 82, 259, 820, and 2600 mg/kg Control group and Treatment: None There were no mortalities at any dosage level tested. The LD50 in albino rabbits is greater than the highest dose tested (approx. 2.6 g/kg body weight). Signs of toxicity included labored respiration and central nervous system depression. All animals recovered within 4-48 hours after the exposure period began. Moderate erythema and edema were observed.
Result	:	LD50 > 2600 mg/kg
Test condition	:	A single dermal application of the test material was made to four groups of four rabbits at doses of 82, 259, 820, and 2600 mg/kg. The results were converted to weight units by means of the specific gravity. The test material was applied to intact abdominal skin and covered with an occlusive covering for 24 hours. Observations for signs of toxicity were made at one, four and 24 hours after compound administration and thereafter for a total of 7 days. Gross necropsies were performed on all animals at the end of the observation period.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Under conditions of this study, Hexanol, branched and linear has a low order of acute dermal toxicity in rabbits.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

03.04.2006 (13)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	Occlusive
Exposure time	:	24 hour(s)

Number of animals	:	16
Vehicle	:	other: none
PDII	:	
Result	:	moderately irritating
Classification	:	
Method	:	other: similar to OECD TG 404
Year	:	1960
GLP	:	
Test substance	:	
Remark	:	A single 24-hour application of Hexanol, branched and linear to intact rabbit skin produced moderate irritation. Skin irritation consisted of slight to moderate erythema, moderate edema, atonia, and desquamation persisted to termination on day 14.
Test condition	:	Hexanol, branched and linear was applied to the clipped, abdominal skin of 4 groups of 4 rabbits. Each application consisted of 0.10, 0.316, 1.00, or 3.16 g/kg test material under an occlusive dressing which was left in place for 24 hours. Measurements were made at 1 hour and at 24, 48 and 72 hours after dressing removal and continued daily for 7 days.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear
Conclusion	:	Under the conditions of the study, Hexanol, branched and linear produced moderate irritation to rabbit skin.
Reliability	:	(2) valid with restrictions Pre-GLP
Flag	:	Critical study for SIDS endpoint

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5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	highly irritating
Classification	:	
Method	:	other: similar to OECD TG 405
Year	:	
GLP	:	
Test substance	:	
Result	:	Median Scores were: 24 hr - 31 72 hr - 23 7 days - 0 Hexyl alcohol caused severe eye irritation involving all eye structures and was based on persistent iritis, corneal opacity, and in two animals, corneal vascularization.
Test condition	:	A single application of 0.1 ml of undiluted alcohol was made into the conjunctival sac of the left eye of each rabbit. The untreated eye served as the control. The treated eye was held closed for 1 second, and eyes were not washed. Observations for irritancy and possible systemic toxicity were made at 1, 4, and 24 hours and at 2, 3, 4, and 7 days. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.
Test substance	:	CAS No. 68526-79-4; Hexanol, branched and linear

Reliability	:	(2) valid with restrictions Pre GLP
Flag	:	Critical study for SIDS endpoint

03.04.2006 (22)

5.3 SENSITIZATION

Type	:	Guinea pig maximization test
Species	:	guinea pig
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	
Method	:	other: Magnusson, B. Kligman, A.M. J. Invest. Dermatol., 52, 1969.
Year	:	1969
GLP	:	
Test substance	:	
Test substance	:	Analogue substance CAS No. 111-27-3; 1-Hexanol
Reliability	:	(1) valid without restriction Peer reviewed publication.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (5)

Type	:	other: Human Maximization (as described by Epstein and Kligman)
Species	:	human
Number of animals	:	
Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: not specified
Year	:	
GLP	:	
Test substance	:	
Remark	:	The test substance was prepared and administered as a 1% solution of 1-hexanol in petrolatum.
Test substance	:	CAS No. 111-27-3, 1-hexanol
Conclusion	:	Not likely to be a skin sensitizer.
Reliability	:	(2) valid with restrictions Peer reviewed publication.
Flag	:	Critical study for SIDS endpoint

03.04.2006 (5)

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rabbit
Sex	:	male/female
Strain	:	other: Albino
Route of admin.	:	dermal
Exposure period	:	10 days
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0 g/kg, 0.4 g/kg and 2.0 g/kg
Control group	:	other: Isopropyl alcohol
NOAEL	:	= 2000 mg/kg
Method	:	other

Year	:	1961
GLP	:	no
Test substance	:	
Remark	:	Duration of test: 12 Days There was no evidence of systemic toxicity at either dose of the test substance. Histopathological findings were unremarkable. Repeated application of the test material to the skin of albino rabbits at both dose levels produced moderate to marked degree of irritation. A slight to marked degree of edema was observed in two low-dose animals and three high-dose animals following one or more of the first three applications. Also, the exposed skin of two high-dose animals showed necrosis.
Result	:	NOAEL for systemic toxicity = 2.0 g/kg
Test condition	:	Undiluted control and test materials were applied to intact skin of the animals. Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each application and at study termination. Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application and brain, liver, kidney, and blood samples were taken. In addition, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved.
Test substance	:	Analogue substance - CAS No. 111-27-3; 1-Hexanol
Conclusion	:	Under the conditions of this study, Hexanol, branched and linear can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

03.04.2006 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium
Test concentration	:	8, 40, 200, 1000, and 5000 micrograms/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1983
GLP	:	yes
Test substance	:	
Test substance	:	Analogue substance - CAS No. 111-27-3, 1-hexanol
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

03.04.2006 (6)

Type	:	Ames test

System of testing	:	Salmonella typhimurium
Test concentration	:	6.25, 25, 100, 400, and 1600 micrograms/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1983
GLP	:	yes
Test substance	:	

Test substance	:	Analogue substance - CAS No. 111-27-3, 1-hexanol
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

03.04.2006 (6)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	19 days
Frequency of treatm.	:	7 hrs/day
Duration of test	:	Gestation days 1-19
Doses	:	3500 mg/m3 (Saturated vapors)
Control group	:	other: 15 sham-exposed rats
NOAEL maternal tox.	:	> 3500 - mg/m³
Method	:	other
Year	:	1989
GLP	:	no data
Test substance	:	other TS

Remark	:	No. of animals/sex/dose: 15 dams/treatment Statistical methods: MANOVA, ANOVA, Kruskal-Wallis test The test substance was administered by inhalation to reflect the route of exposure found in industry. However, due to the low volatility of the alcohols, concentrations sufficient to induce maternal toxicity could not be achieved. There were no significant fetal malformations associated with inhalation of 1-hexanol by the dam. There was a slight but statistically significant increase in resorptions (1.3 vs. 0.4 per litter for controls). However, this resorption mean was still in the range seen in historical controls.
Result	:	NOAEL > 3500 mg/m3
Test condition	:	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the

test substance was ³ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.

Test substance : 1-Hexanol
Conclusion : Inhalation of saturated vapors of 1-hexanol is not maternally toxic or teratogenic in rats.
Reliability : (2) valid with restrictions
2 - Reliable with restrictions.

28.11.2001 (1)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 68526-83-0
CAS No.	:	68526-83-0
EINECS Name	:	Alcohols, C7-9-iso-, C8-rich
EC No.	:	271-231-4
TSCA Name	:	Alcohols, C7-9-iso-, C8-rich

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.09.2001
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	05.04.2006
Revision date	:	
Date of last update	:	05.04.2006
Number of pages	:	43
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C8H18O
Molecular weight : 130.23
Petrol class :

Flag : Critical study for SIDS endpoint
04.04.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 104-76-7
IUPAC Name: 2-ethylhexan-1-ol
R Length (C number): C8
Structure of R: Branched and Linear
Category Member: No (analogue substance used for supporting information)

CAS RN: 111-87-5
IUPAC Name: octan-1-ol
R Length (C number): C8
Structure of R: Linear
Category Member: No (analogue substance used for supporting information)

CAS RN: 68526-83-0
IUPAC Name: Alcohols, C7-C9-iso, C8 rich
R Length (C number): C8
Structure of R: Branched, primarily methyl branched (isomeric structures)
Category Member: Yes

04.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Exxal 8

21.09.2004

isooctanol

21.09.2004

isooctyl alcohol

21.09.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	68526-83-0
EC-No	:	271-231-4
EINECS-Name	:	Alcohols, C7-9-iso-, C8-rich
Molecular formula	:	C8H18O

Value : = 99 % w/w

Remark : Commercial product typically consists of methyl-1-heptanols and/or dimethyl-1-hexanols.

04.04.2006

1.4 ADDITIVES

Purity type : typical for marketed substance
CAS-No :
EC-No :
EINECS-Name :
Molecular formula :
Value :
Function of additive :

Remark : No additives present.
04.04.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Priciple use of these alcohols is in the preparation of plasticizers, mainly dioctyl phthalate, but also esters of adipic, sebacic, azelmic, and trimellitic acids. Also used as a solvent for fats, oils, and waxes, as well as various rubber formulations and resins.

04.04.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -65 °C
Sublimation	:	
Method	:	other: ASTM D97
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (12)

2.2 BOILING POINT

Value	:	= 185 - 193 °C at 1013 hPa
Decomposition	:	
Method	:	other: D1078/01
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (12)

2.3 DENSITY

Type	:	density
Value	:	= .831 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(4) not assignable Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

21.09.2004 (12)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 2.59 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable. Value was provided by the experimental database of the EPIWIN program.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (20)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 2.9 - 3.4 at 30 °C
pH value	:	
Method	:	OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1998
GLP	:	yes
Test substance	:	
Remark	:	Test Type: N-Octanol/Water Partition Coefficient (HPLC method)
Result	:	The test substance eluted as several groups. The three major components C7, C8, C9 alcohols had Log Pow values of 2.9, 3.0, and 3.4 respectively. The retention time for the 3 major components were 5.72, 6.03, and 7.28 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Test condition	:	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

04.04.2006 (7)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 1379 - 1485 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (22)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 60 °C
Type	:	closed cup
Method	:	other: TCC ASTM D56
Year	:	
GLP	:	no data
Test substance	:	other TS

Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(4) not assignable Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.
Flag	:	Critical study for SIDS endpoint

21.09.2004 (12)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.50 at 25°C
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.04.2006 (17)

2.13 VISCOSITY

Value	:	= 13 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	
GLP	:	no data
Test substance	:	other TS
Remark	:	Value measured in cSt
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(4) not assignable Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.

21.09.2004 (12)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (11)

Type :
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000
Rate constant : = .000000000000125338 cm^3/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year :
GLP :
Test substance :

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
10.2	12.53 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition	:	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life for the test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (21)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other: Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.
Result	:	Hydolysis as a Function of Molecular Structure Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis. Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982). References: Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press, Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.
Flag : Critical study for SIDS endpoint
20.03.2006 (10)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 130.23 g/mol
Water solubility = 1379 mg/L
Vapour pressure = 2.59 Pa
log Kow = 3.20
Melting point = -65 deg C

Degradation half-lives:

Air - 10.2 hrs
Water - 120 hrs
Soil - 720 hrs
Sediment - 7200 hrs

This model was run assuming 100% discharge to water.

Result : Air - 0.03%
Water - 96.6%
Soil - 0.03%
Sediment - 3.3%

Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (19)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 130.23 g/mol Water solubility = 1379 mg/L Vapour pressure = 2.59 Pa log Kow = 3.20 Melting point = -65 deg C
Result	:	Air - 2.0% Water - 40.2 % Soil - 56.5% Sediment - 1.3% Suspended Sed - 0.04% Biota - <0.01%
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

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3.3.2 DISTRIBUTION

Media	:	other: Koc
Method	:	other (calculation)
Year	:	2003
Method	:	The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980). PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases

in soil, or between water and sediment in aquatic ecosystems.

Result : Koc = 23.7
log Koc = 1.37

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured. The value was calculated based on chemical structure as modeled by EPIWIN.

Flag : Critical study for SIDS endpoint

05.04.2006 (18) (23)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Contact time : 28 day(s)
Degradation : = 82 (±) % after 28 day(s)
Result :
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1997
GLP : yes
Test substance :

Remark : Test Type: Manometric Respirometry Test
Result : Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 82% degradation of the test material was observed. 10% biodegradation was achieved on day 3.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	84.7, 77.1, 84.0	82.0
Na Benzoate	91.3, 81.3	86.3

* replicate data

Test condition : Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 51 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich

Conclusion : Test substance is readily biodegradable.
Reliability : (1) valid without restriction
05.04.2006 (8)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 14 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: no data
Year	:	1986
GLP	:	no data
Test substance	:	

Method : Trimmed Spearman Karber Method

Result : 96 hour LC50 = 14.0 mg/L (95% CI 13.6 to 14.5) based upon measured values

Analytical method used was Gas-Liquid Chromatography.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
8.8	0
10.7	1
12.7	2
16.5	20
20.4	20

* 20 fish added at test initiation

Test condition : Treatment solutions were prepared by diluting a 275mg/L stock solution. Nominal octanol treatment levels were 8.6, 10.8, 13.5, 16.9, 21.1mg/L, which measured 8.8, 10.7, 12.7, 16.5, and 20.4mg/L, respectively. Control/dilution water was EPA Duluth laboratory water. Twenty fish were tested per treatment. Treatment volume = 2.0L. Test parameters were as follows: temperature=25.3 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 28 days old; fish mean wt = 0.075g; fish mean length = 16.5mm; fish loading = 0.75g/L/day. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

05.04.2006 (13)

Type	:	other: calculated
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 19.9 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a

subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C8 alcohol with a Kow of 2.73.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion : Based on the calculated Kow value, the C8 alcohol is expected to have an acute 96-hour LC50 of 19.9 mg/L and a Chronic Value of 2.9 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.04.2006 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = 31.8
Limit Test : no
Analytical monitoring : no
Method : other: US EPA 660/3-75-009
Year : 1980
GLP : no data
Test substance :

Method : Spearman-Karber (Finney, D.J., 1971)
Remark : Test Type: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
Result : 48-hour LC50 = 31.8 mg/L (CI 26.5 - 38.2) as Total Carbon, based upon nominal concentrations.

Nominal Conc.	% Mortality @ 48 hr.
Control	0
10 mg/L	10
18 mg/L	20
32 mg/L	25
56 mg/L	95
100 mg/L	100
180 mg/L	100

Test condition : Individual treatments were prepared by adding varying amounts of test material directly to 250 mL of dilution water in glass beakers. Nominal test concentrations were 10, 18, 32, 56, 100 and 180 mg/L. Four replicates were prepared for each treatment and control. Five daphnids per replicate chamber. Test placed in a temperature-controlled waterbath at 20.5 to 21.0 Deg. C. The test was performed under static conditions.

Lighting was 16 hours light : 8 hours dark. Dissolved oxygen ranged from 8.6 to 9.6 mg/L during the study. The pH was ranged from 7.8 to 8.4 during the study. Dilution water hardness was 240 mg/L as CaCO3, alkalinity was 145 mg/L as CaCO3, and conductivity was 600 µmhos/cm. Organisms were supplied by in-house cultures. Age = <20 hours old.

Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Test substance is considered to have moderate acute toxicity.
Reliability	:	(2) valid with restrictions Analytical verification not performed, quality assurance unknown.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (26)

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 22.4 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C8 alcohol with a Kow of 2.73.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Based on the calculated Kow value, the C8 alcohol is expected to have an acute 48-hour EC50 of 22.4 mg/L and a Chronic Value of 1.6 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.04.2006 (4)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green alga
Endpoint	:	biomass
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 14.6 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C8 alcohol with a Kow of 2.73.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion : Based on the calculated Kow value, the C8 alcohol is expected to have an acute 96-hour EC50 of 14.6 mg/L and a Chronic Value of 2.2 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.04.2006 (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species : other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint : other: LC50
Exposure period : 30 day(s)
Unit : mg/l
ChV : = 2.9 calculated
Method : other: calculated
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C8 alcohol with a Kow of 2.73.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion : Based on the calculated Kow value, the C8 alcohol is expected to have a 30-day Chronic Value of 2.9 mg/L
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.04.2006 (4)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia sp. (Crustacea)
Endpoint :
Exposure period : 16 day(s)
Unit : mg/l
EC50 : = 1.6 calculated

Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C8 alcohol with a Kow of 2.73.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Based on the calculated Kow value, the C8 alcohol is expected yo have a 16-day EC50 of 1.6 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (4)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: Earthworm
Endpoint	:	
Exposure period	:	14 day(s)
Unit	:	mg/kg soil dw
LC50	:	= 477 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C8 alcohol with a Kow of 2.73.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Based on the calculated Kow value, the C8 alcohol is expected to have a 14-day EC50 of 477 mg/kg soil.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (4)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: None
Doses	:	
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1988
GLP	:	yes
Test substance	:	
Remark	:	Following dosing, the following symptoms were observed: sedation, ventral body position in males, hunched posture, and ruffled fur. However, all animals had recovered within 6 days of dosing. At necropsy, no macroscopic abnormalities were observed. Route of administration: Oral gavage Frequency of Treatment: Single dose Dose/Concentration Levels: 2000 mg/kg
Result	:	LD50 > 2000 mg/kg
Test condition	:	After being fasted for 12 to 18 hours, animals were administered a single oral gavage dose of 2,000 mg/kg of the undiluted test article. Observations were made four times on day 1; and daily for 14 days.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Under the conditions of this study, Alcohols, C7-9 branched has a low order of toxicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.04.2006 (24)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 200 ppm
Species	:	rat
Strain	:	Wistar
Sex	:	male
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Inhalation Frequency of Treatment: Single 6 hour exposure Dose/Concentration Levels: Saturated Vapors There were no deaths during the treatment period. There were no apparent signs of toxicity or alterations to behavior other than blinking in

rats. No macroscopic abnormalities were observed at necropsy.

Result	:	LC50 > 200 ppm
Test condition	:	Rats were exposed to near-saturation levels (200 ppm) of vapors of Alcohols, C7-9 branched in a 500 L stainless steel inhalation chamber for 6 hours. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml of the test substance. Air flow through each bubbler was 18 l/m, and the total flow through the chamber was 36 l/m. Actual chamber concentration was not measured; theoretical chamber concentration was calculated to be 200 ppm. Animals were observed at one-hour intervals during the exposure. Animals were observed 24 hours following exposure and then necropsies were performed.
Conclusion	:	Under the conditions of this study, Alcohols, C7-9 branched has a low order of acute inhalation toxicity in rats.
Reliability	:	(2) valid with restrictions No analysis of exposure atmosphere.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (16)

Type	:	LC50
Value	:	> 200 ppm
Species	:	mouse
Strain	:	Swiss
Sex	:	male
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Inhalation Frequency of Treatment: Single 6 hour exposure Dose/Concentration Levels: Saturated Vapors There were no deaths during the treatment period. There were no apparent signs of toxicity or alterations to behavior other than blinking in mice. No macroscopic abnormalities were observed at necropsy.
Result	:	LC50 > 200 ppm
Test condition	:	Mice were exposed to near-saturation levels (200 ppm) of vapors of Alcohols, C7-9 branched in a 500 L stainless steel inhalation chamber for 6 hours. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml of the test substance. Air flow through each bubbler was 18 l/m, and the total flow through the chamber was 36 l/m. Actual chamber concentration was not measured; theoretical chamber concentration was calculated to be 200 ppm. Animals were observed at one-hour intervals during the exposure. Animals were observed 24 hours following exposure and then necropsies were performed.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Under the conditions of this study, Alcohols, C7-9 branched has a low order of acute inhalation toxicity in mice.
Reliability	:	(2) valid with restrictions No analysis of exposure atmosphere.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (16)

Type	:	LC50
Value	:	> 200 ppm
Species	:	guinea pig
Strain	:	other: English short hair

Sex	:	male
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	Route of administration: Inhalation Frequency of Treatment: Single 6 hour exposure Dose/Concentration Levels: Saturated Vapors There were no deaths during the treatment period. There were no apparent signs of toxicity or alterations to behavior. No macroscopic abnormalities were observed at necropsy.
Result	:	LC50 > 200 ppm
Test condition	:	Guinea pigs were exposed to near-saturation levels (200 ppm) of vapors of Alcohols, C7-9 branched in a 500 L stainless steel inhalation chamber for 6 hours. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml of the test substance. Air flow through each bubbler was 18 l/m, and the total flow through the chamber was 36 l/m. Actual chamber concentration was not measured; theoretical chamber concentration was calculated to be 200 ppm. Animals were observed at one-hour intervals during the exposure. Animals were observed 24 hours following exposure and then necropsies were performed.
Test substance	:	CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion	:	Under the conditions of this study, Alcohols, C7-9 branched has a low order of acute inhalation toxicity in guinea pigs.
Reliability	:	(2) valid with restrictions No analysis of exposure atmosphere.
Flag	:	Critical study for SIDS endpoint

05.04.2006 (16)

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5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2623 mg/kg bw
Species	:	rabbit
Strain	:	other: Albino
Sex	:	male/female
Number of animals	:	8
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	Animals in the 83, 262, and 820 mg/kg dose groups exhibited normal appearance and behavior throughout the study. At the highest dose (2623 mg/kg), animals exhibited labored respiration and were inactive. One animal in the high dose group died within 24 hours. The remaining animals in this dose group returned to normal appearance and behavior 2 days after the treatment. Route of administration: Dermal; with occlusive binding

Frequency of treatment: Single 24 hour exposure
Dose/Concentration Levels: 83, 262, 820, 2623 mg/kg (undiluted)
Control group and treatment: None

Result : Dermal LD50 > 2623 mg/kg
Test condition : The test substance was applied dermally to rabbits (4/sex/dose) under occlusive binding and removed after 24 hours. The results were converted to weight units by means of the specific gravity. Animals were observed 1, 4, and 24 hours after initial application of Alcohols, C7-9 branched and once daily for the next 7 days. At the termination of the study, survivors were weighed and gross necropsies were performed.
Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion : Alcohols, C7-9 branched showed a low order of acute dermal toxicity under the conditions of this study.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
05.04.2006 (16)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure : Occlusive
Exposure time : 4 hour(s)
Number of animals : 16
Vehicle :
PDII : 3.08
Result : moderately irritating
Classification :
Method : other: similar to OECD TG 404
Year : 1960
GLP :
Test substance :

Remark : A single 4-hour application of Alcohols, C7-9-iso, C8 rich to intact rabbit skin produced moderate irritation. Skin irritation consisted of slight to moderate erythema, moderate edema, atonia, and desquamation persisted to termination on day 14.

The single 4-hour application resulted in a primary irritation index of 3.08. Mean scores at 24, 48, and 72-hours were 1.83, 1.83, and 2.0 for erythema and 0.83, 1.33, and 1.5 for edema.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion : Under the conditions of the study, Alcohols, C7-9-iso, C8 rich produced moderate irritation to rabbit skin.
Reliability : (2) valid with restrictions
Pre-GLP
Flag : Critical study for SIDS endpoint
05.04.2006 (15) (25)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : .1 undiluted
Dose :
Exposure time :

Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	highly irritating
Classification	:	
Method	:	other: similar to OECD TG 405
Year	:	
GLP	:	
Test substance	:	

Result : Median Scores were:

24 hr - 26
72 hr - 18
7 days - 0

Iso-octyl alcohol produced persistent, widespread corneal opacity which generally cleared within 7 days.

Test condition : A single application of 0.1 ml of undiluted alcohol was made into the conjunctival sac of the left eye of each rabbit. The untreated eye served as the control. The treated eye was held closed for 1 second, and eyes were not washed. Observations for irritancy and possible systemic toxicity were made at 1, 4, and 24 hours and at 2, 3, 4, and 7 days. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich

Reliability : (2) valid with restrictions
Pre GLP

Flag : Critical study for SIDS endpoint

05.04.2006 (25)

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	highly irritating
Classification	:	
Method	:	other: similar to OECD TG 405
Year	:	
GLP	:	
Test substance	:	

Result : Median Scores were:

24 hr - 19
72 hr - 20
7 days - 0

2-ethylhexyl alcohol produced persistent, widespread corneal opacity which generally cleared within 7 days.

Test condition : A single application of 0.1 ml of undiluted alcohol was made into the conjunctival sac of the left eye of each rabbit. The untreated eye served as the control. The treated eye was held closed for 1 second, and eyes were not washed. Observations for irritancy and possible systemic toxicity were made at 1, 4, and 24 hours and at 2, 3, 4, and 7 days. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.

Test substance : Analogue substance: CAS No. 104-76-7; 2-ethylhexan-1-ol

Reliability : (2) valid with restrictions

Pre-GLP

05.04.2006 (25)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	3 months
Frequency of treatm.	:	daily (5 days /week)
Post exposure period	:	none
Doses	:	25, 125, 250, 500 mg/kg (in aqueous emulsion)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 125 mg/kg
LOAEL	:	= 250 mg/kg
Method	:	
Year	:	1990
GLP	:	yes
Test substance	:	
Remark	:	Vehicle: bidistilled water containing 5 ug/ml Cremophor EL. Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed and samples of liver tissues and bone marrow were prepared for electron microscopy investigations; liver homogenates were prepared for clinicochemical examinations.
Result	:	Result: Limited study: The oral administration of 2-ethylhexanol over a period of 3 months led to an impairment of feed consumption and body weight gain in the male and female animals of the 500 mg/kg dose group. The cyanide-insensitive palmitoyl CoA-oxidation in the liver of male and female rats was strongly induced in the 500 mg/kg dose group and less pronounced in the 250 mg/kg dose group, probably due to a proliferation of peroxisomes. No substance-related findings were observed in the other dose groups. NOEL: 125 mg/kg bodyweight LOEL: 250 mg/kg bodyweight Main study: Per dose group 10 male and 10 female rats were treated. After the 3-month administration of 2-ethylhexanol toxic effects occurred in male and female rats of the 500 and 250 mg/kg dose groups. Typical findings were: 25 and 125 mg/kg groups: no substance-related findings 250 mg/kg group: increased relative liver weights in both sexes; increased relative stomach weights in females;

decrease in alkaline phosphatase and glucose in males; decrease in alanine-aminotransferase in female rats.

500 mg/kg group: increased relative liver and stomach weights in both sexes; increased relative liver weights in the animals of both sexes; increased absolute stomach weights in female rats; decrease in alanine-aminotransferase, glucose and cholesterol in both sexes; decrease in alkaline phosphatase in males; single or multiple slightly elevated foci in the mucosa of the forestomach of male and female rats; focal or multifocal acantosis in the mucosa of the forestomach of one male and five female animals.

Test substance : Analogue substance: CAS No. 104-76-7; 2-ethylhexan-1-ol
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
05.04.2006 (2)

Type :
Species : rat
Sex : male
Strain : Wistar
Route of admin. : other: oral gavage
Exposure period : 14 days
Frequency of treatm. : once/day
Post exposure period :
Doses :
Control group :
NOAEL : = 130 mg/kg bw
Method : other: NA
Year : 1984
GLP : no data
Test substance :

Remark : Iso-octanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Iso-octanol did not induce any changes in glycogen vacuolation or fat vacuolation. The activity of peroxisome-associated enzymes and levels of cholesterol and triglyceride were not significantly different between animals treated with iso-octanol and vehicle controls. No hyperlipidemia was observed.
No. of animals/sex/dose: 5/treatment, 10/control; 1mmol/kg/day of iso-octanol (130 mg/kg/day)
Vehicle: Polyethylene glycol 300
Statistics: Mean values compared to controls by Student's t-test.
Result : NOAEL = 130 mg/kg/day
Test condition : After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined.
Test substance : Iso-octanol
CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich
Conclusion : Under the conditions of this study, iso-octanol had a low order of sub-acute toxicity in male rats for the endpoints studied.
Reliability : (2) valid with restrictions
Not a guideline study.
05.04.2006 (3)

Type	:	
Species	:	rabbit
Sex	:	male/female
Strain	:	other: Albino
Route of admin.	:	dermal
Exposure period	:	10 days
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0.4 g/kg and 2.0 g/kg
Control group	:	other: Isopropyl alcohol, 2/sex
NOAEL	:	= 2000 mg/kg
Method	:	other
Year	:	1961
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Not specified
Remark	:	Animals in all exposure groups displayed normal appearance and behavior throughout the study. Although a slight decrease in body weight was observed initially, animals regained weight by the end of the study. Repeat application of the control substance, isopropyl alcohol produced slight irritation characterized by slight to moderate erythema, atonia, and desquamation. Repeated application of Alcohols, C7-9 branched resulted in moderate to severe irritation. Fissuring and coriaceous skin were also observed at both the low and high dose levels. Necrosis was observed in the high dose animals as well. Clinical studies did not indicate any other signs of toxicity. There was a general increase in the hematocrit and erythrocyte values at the end of the study. Duration of test: 12 days Number of animals: 8 rabbits (2/sex/dose)
Result	:	NOAEL for systemic toxicity = 2.0 g/kg
Test condition	:	Undiluted control and test materials were applied to intact skin of the animals (2/sex/dose). Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each exposure and at study termination. Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved.
Conclusion	:	Under the conditions of this study, Alcohols, C7-9 branched can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study.
Reliability	:	(2) valid with restrictions 2 - Valid with restrictions

28.11.2001 (5)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	S. typhimurium, E. coli

Test concentration	:	1, 5, 10, 50, 100, 500, and 1000 ug/plate.
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	negative
Method	:	other
Year	:	1985
GLP	:	no data
Test substance	:	
Method	:	Samples were run in duplicate. No further details provided.
Remark	:	Strain: Salmonella typhimurium /TA98; TA100; TA1535; TA1537; TA1538; E. coli WP2uvrA Metabolic Activation: S9 mixture
Result	:	In all of the strains tested, there was no evidence of mutagenicity of 2-ethyl-1-hexanol in the presence or absence of metabolic activation. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 2-ethyl-1-hexanol samples.
Test condition	:	2-Ethyl-1-hexanol (98% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (Polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)-acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls.
Test substance	:	2-Ethyl-1-hexanol (CAS No. 104-76-7)
Conclusion	:	2-Ethyl-1-hexanol is not mutagenic in bacteria under the conditions of this study.
Reliability	:	(2) valid with restrictions (Similar to OECD 471)

05.04.2006 (14)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	male
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	5 days
Doses	:	0.02, 0.07, 0.21 ml/kg day
Result	:	
Method	:	other: as described by author
Year	:	1981
GLP	:	yes
Test substance	:	
Result	:	Result: Groups of 5 male F-344 rats were treated with 2-ethylhexanol. Of the 50 metaphase bone marrow cells examined from each animal, no significant increase in chromatid and chromosome breaks or structural rearrangements was noted. In addition, the mitotic index was unaffected by 2-ethylhexanol. At the dose levels tested 2-ethylhexanol did not induce detectable chromosomal aberrations after oral administration.
Test substance	:	Analogue substance: CAS No. 104-76-7; 2-ethylhexan-1-ol
Reliability	:	(1) valid without restriction

Flag	:	Critical study for SIDS endpoint
05.04.2006		(6)
Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	i.p.
Exposure period	:	single administration
Doses	:	456 mg/kg
Result	:	
Method	:	other: as described by author
Year	:	1982
GLP	:	yes
Test substance	:	
Result	:	B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.
Test substance	:	Analogue substance: CAS No. 104-76-7; 2-ethylhexan-1-ol
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint
05.04.2006		(6)

5.7 CARCINOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	24 months
Frequency of treatm.	:	5 days/week
Post exposure period	:	none
Doses	:	0, 50, 150, 500 mg/kg
Result	:	
Control group	:	yes, concurrent vehicle
Method	:	other: according to EPA-TSCA guidelines
Year	:	
GLP	:	yes
Test substance	:	
Remark	:	Vehicle: aqueous 0.005% Cremophor EL. In addition to the vehicle control groups, 50 rats/sex were dosed with water; Concurrently to the main study, a satellite study was performed. 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 500 mg/kg. One group of rats (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 18 months and then sacrificed. Another group (50 rats/sex; recovery group) was treated with the same dose for 18 months and thereafter with vehicle only for 6 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female rats received the vehicle for 18 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.

Result	:	Result: Satellite study: In the interim sacrifice group a reduced body weight gain (both sexes) and clinical symptoms like poor general condition, labored breathing and "genital region smeared with urine" (females only) was observed. A slightly increased mortality in females was observed. The relative weight of testes and brain (males), stomach (females), liver and kidney (both sexes) were increased. In the recovery group similar effects were observed. After termination of treatment the body weight gain increased indicating a recovery effect. 18 males and 17 females died prematurely and one each had a focal hyperplasia in the forestomach. In the glandular stomach erosions were seen in 4 males and females each. Glandular cysts occurred in 6 males and 8 females. Main study: 2-Ethylhexanol was not oncogenic in the rat under the conditions of this assay. In both sexes the sum of primary tumors, the sum of benign tumors and the sum of malignant tumors was lower in the top dose group than in either the vehicle control or the water control groups.
Test substance	:	Analogue substance: CAS No. 104-76-7; 2-ethylhexan-1-ol
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.04.2006 (6)

Species	:	mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	gavage
Exposure period	:	18 months
Frequency of treatm.	:	5 days/week
Post exposure period	:	none
Doses	:	0, 50, 200, 750 mg/kg
Result	:	
Control group	:	yes, concurrent vehicle
Method	:	other: according to EPA-TSCA guidelines
Year	:	
GLP	:	yes
Test substance	:	

Remark	:	Vehicle: aqueous 0.005% Cremophor EL In addition to the vehicle control groups, 50 mice/sex were dosed with water. Concurrently to the main study, a satellite study was performed: 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 750 mg/kg. One group of mice (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 13 months and then sacrificed. Another group (50 mice/sex; recovery group) was treated with the same dose for 13 months and thereafter with vehicle only for 5 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female mice received the vehicle for 13 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.

Result	:	Result: Satellite study: The administration of 2-ethylhexanol to male and female mice for 13 months at a dose of 750 mg/kg caused increased mortality, reduced feed consumption and body weight gain in both sexes. The body weight gain of male and female animals of the recovery group were reduced as long as the animals were treated. After termination of treatment the male animals gained weight and reached nearly the values of the control group, indicating a recovery effect. No such effect was seen in females. Pathology revealed some statistically significant changes in organ weights and masses of foci in liver and stomach. One male and one female animal of the recovery group which died premarurely had a focal hyperplasia in the forestomach. Main study: 2-Ethylhexanol was not oncogenic in the mouse under the conditions of this assay. A slight increase in the incidence of hepatocellular carcinoma in the females of the high dose group was statistically significant if compared to the control group dosed with the emulsion vehicle, but not when compared to the control group dosed with water. This difference was regarded as incidental and not biologically relevant, based upon comparison with published data, and because of the lack of metastases. No statistically significant increase in tumor incidence occured in male mice.
Test substance	:	Analogue substance: CAS No. 104-76-7; 2-ethylhexan-1-ol
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.04.2006 (6)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	Gestation days 1-19
Frequency of treatm.	:	7 hrs/day
Duration of test	:	19 days
Doses	:	400 mg/m3
Control group	:	other: 15 sham-exposed rats
NOAEL maternal tox.	:	>= 400 mg/m³
Method	:	other
Year	:	1989
GLP	:	no data
Test substance	:	
Method	:	MANOVA, ANOVA, Kruskal-Wallis test
Remark	:	No treatment-related effects were observed in dams. There were no

significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups.
No. of animals/sex/dose: 15

Result : Maternal and Developmental NOAEL >= 400 mg/m3

Test condition : Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ³ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heat compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m3. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO2 asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.

Test substance : 1-Octanol

Conclusion : Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Octanol does not induce maternal or fetal toxicity.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

05.04.2006 (1)

Species : rat

Sex : female

Strain : Sprague-Dawley

Route of admin. : other: oral gavage

Exposure period : GD 6-15

Frequency of treatm. :

Duration of test :

Doses : 100, 500, and 1000 mg/kg/day

Control group : other: Carrier only - corn oil

NOAEL maternal tox. : = 500 - mg/kg bw

Method : OECD Guide-line 414 "Teratogenicity"

Year : 1994

GLP : yes

Test substance :

Method : Nested analysis of covariance, Least Significant Difference (LSD), Chi-square, Fisher Exact test, Armitage's test.

Remark : No. of animals/dose: 25
One animal in the high dose group was euthanized in moribund condition on GD 9. The animal had extreme abdominal staining just prior to death, but there were no significant findings at postmortem examination and the cause of morbidity was therefore not established. Adverse clinical signs were observed in 8 of the 24 dams in the high dose group. These signs included emaciation, decreased food consumption, abdominal/anogenital staining, rales, hypoactivity, and little or no stool. The symptoms were transient and generally were not observed following cessation of dosing. The remaining dams in the high dose group had incidental findings such as alopecia, but otherwise appeared normal throughout the study. There were no observable abnormalities in dams of the middle and low dose groups

throughout the gestational period. In the high dose group, statistically significant decreased body weight gain and food consumption were observed from GD 6-9 and GD6-15 compared to controls. However, these effects subsided after cessation of treatment and body weight and food consumption for the overall gestational period (GD 6-21) were not significantly different between the high dose group and controls. There were no maternal findings at necropsy that were judged to be the result of treatment with Alcohols, C7-9 branched. For the most part, uterine implantation parameters were equivalent between the treated and control groups.

There were slight differences between the high dose group and the control group in the number of post-implantation losses and resorptions, however these differences were not statistically significant and were deemed to be due to the poor health of the dams.

Mean fetal body weight was equivalent between treated and control fetuses of both sexes. Three low dose, two mid dose, and one high dose fetus were stunted. There were no statistically significant differences in mean skeletal ossification sites and in total or individual external, visceral, or skeletal malformations between control and treated groups. There were statistically significant increases in total fetuses with skeletal variations and in the incidence of hypoplastic skull bones in the high dose group when compared to controls. These findings were slightly higher than the historical control range of the lab and were not observed with litter-based analysis. Statistically significant increases in the number of lumbar ribs were observed in the middle and high dose groups. However, due to the lack of embryotoxicity observed in this study, these findings were attributed to maternal toxicity observed during treatment.

Result : Maternal NOAEL = 500 mg/kg/day
Fetal NOAEL = 1000 mg/kg/day

Test condition : Mated females were assigned to dose groups of 100, 500, and 1000 mg/kg/day or to a corn oil-only group (25/dose). The test substance was administered in volumes of 5 ml/kg. Body weight and food consumption measurements were made on GD 0, 6, 9, 12, 15, 18, and 21. The animals were examined for viability twice daily during the treatment period and once daily thereafter. Clinical observations were made daily during gestation. On GD 21, animals were sacrificed and cesarean sections and necropsies were performed. Uterine weights with ovaries attached were recorded, uterine contents were examined, and implantation data were recorded. All live fetuses were weighed, sexed externally, and examined externally for gross malformations. Approximately one-half of the fetuses were prepared for examination of abnormalities in the head and the other half were preserved for examination of skeletal abnormalities.

Test substance : CAS No. 68526-83-0; Alcohols, C7-9-iso, C8-rich

Conclusion : Under the conditions of this study, Alcohols, C7-9 branched induces maternal toxicity at concentrations that are not embryotoxic.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

05.04.2006 (9)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 70914-20-4
Memo	:	HPV Chemical
CAS No.	:	70914-20-4
TSCA Name	:	Alcohols, C6-8-branched
Molecular Formula	:	Unspecified

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.11.2001

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.11.2001
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	04.04.2006
Revision date	:	
Date of last update	:	04.04.2006
Number of pages	:	35
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C7H16O
Molecular weight : 116.21
Petrol class :

Flag : Critical study for SIDS endpoint
04.04.2006

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 70914-20-4
IUPAC Name: Alcohols, C6-8 branched
R Length (C number): C7
Structure of R: Branched, primarily methyl branched (isomeric structures)
Category Member: Yes

04.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Exxal 7

20.09.2004

isoheptanol

20.09.2004

isoheptyl alcohol

20.09.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	70914-20-4
EC-No	:	
EINECS-Name	:	Alcohols, C6-8 branched
Molecular formula	:	C7H16O
Value	:	= 98 % w/w

Remark : Commercial product typically consists of methyl-1-hexanols.
04.04.2006

1.4 ADDITIVES

Purity type	:	typical for marketed substance
CAS-No	:	
EC-No	:	
EINECS-Name	:	
Molecular formula	:	

Value :
Function of additive :

Remark : No additives present.
04.04.2006

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Chemical industry: used in synthesis

Remark : Primarily used as a chemical intermediate in the production of ester compounds, such as phthalate plasticizers and esters of carboxylic acid. Also used as solvents or solubilizers in paint and printing inks, as a component in textile auxiliaries and pesticides, for hormone extraction and in the surfactant field as foam boosters or antifrothing agents.

04.04.2006

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -37.2 °C
Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

20.09.2004 (18)

2.2 BOILING POINT

Value	:	= 167 - 176 °C at 1013 hPa
Decomposition	:	
Method	:	other: D1078/01
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (13)

2.3 DENSITY

Type	:	density
Value	:	= .827 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (13)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .58 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (18)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 1.8 - 2.6 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Method	:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (20)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 3539 - 11950 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	no data
Test substance	:	
Method	:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (21)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 60 °C
Type	:	closed cup
Method	:	other: TCC ASTM D56
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(4) not assignable Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (13)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.50 at 25°C
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.04.2006 (15)

2.13 VISCOSITY

Value	:	= 9.4 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered to be reliable.

04.04.2006 (13)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (12)

Type :
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm^3
Rate constant : = .000000000000111208 cm^3/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year :
GLP :
Test substance :

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
11.5	11.12 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition	:	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life for the test substance.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (19)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other: Technical Discussion
Year	:	
GLP	:	
Test substance	:	

Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.
Result	:	Hydolysis as a Function of Molecular Structure Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis. Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982). References: Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press, Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.
Flag : Critical study for SIDS endpoint
20.03.2006 (10)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 116.21 g/mol
Water solubility = 4089 mg/L
Vapour pressure = 0.58 Pa
log Kow = 2.24
Melting point = -37.2 deg C

Degradation half-lives:

Air - 11.5 hrs
Water - 120 hrs
Soil - 720 hrs
Sediment - 7200 hrs

This model was run assuming 100% discharge to water.

Result : Air - <0.01%
Water - 99.4%
Soil - 0.02%
Sediment - 0.5%

Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (17)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2003
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 116.21 g/mol Water solubility = 4089 mg/L Vapour pressure = 0.58 Pa log Kow = 2.24 Melting point = -37.2 deg C
Result	:	Air - 0.3% Water - 67.0 % Soil - 13.3% Sediment - 0.3% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (17)

3.3.2 DISTRIBUTION

Media	:	other: Koc
Method	:	other (calculation)
Year	:	2003
Method	:	The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980). PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases

in soil, or between water and sediment in aquatic ecosystems.

Result : Koc = 12.85
log Koc = 1.11

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured. The value was calculated based on chemical structure as modeled by EPIWIN.

Flag : Critical study for SIDS endpoint

04.04.2006 (16) (22)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 34.5 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: no data
Year	:	1985
GLP	:	no data
Test substance	:	

Method : Trimmed Spearrman Karber Method

Result : 96 hour LC50 = 34.5 mg/L (95% CI 33.1 to 36.0) based upon measured values

Analytical method used was Gas-Liquid Chromatography.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
12.5	0
18.1	1
28.5	0
43.6	20
70.8	20

* 20 fish added at test initiation

Test condition : Treatment solutions were prepared by diluting a 1400mg/L stock solution.

Nominal heptanol treatment levels were 12.5, 19.3, 29.7, 45.7, 70.3mg/L, which measured 12.5, 18.1, 28.5, 43.6, and 70.8mg/L, respectively.

Control/dilution water was EPA Duluth laboratory water.
Twenty fish were tested per treatment. Treatment volume = 2.0L. Test parameters were as follows: temperature=25.6 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 31 days old; fish mean wt = 0.100g; fish mean length = 18.1mm; fish loading = 1.0g/L/day.

Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.04.2006 (14)

Type	:	other: calculated
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 51.2 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical

structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C7 alcohol with a Kow of 2.24.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion : Based on the calculated Kow value, the C7 alcohol is expected to have an acute 96-hour LC50 of 51.2 mg/L and a Chronic Value of 6.9 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.04.2006 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 63
Limit Test : no
Analytical monitoring : no
Method : other: Concept rules of the Dutch Standardization Institute (Adema, 1978)
Year : 1978
GLP : no data
Test substance :

Method : No Data
Remark : Test Type: Daphnid Acute Toxicity Test
Result : 48-hour EC50 = 63 mg/L, based upon nominal concentrations of the test chemicals.
Test condition : Tests using 15 different chemicals, including n-Heptanol, were performed at two different laboratories. Lab I was the National Institute of Public Health, Bilthoven, The Netherlands; Lab II was the Central Laboratory, T.N.O., Delft, The Netherlands. The tests were conducted using standardized tests methods proposed by the Dutch Standardization Institute (Adema, 1978). The tests were conducted in duplicate to determine the reproducibility of the results.

Organisms were supplied by in-house cultures. Age = <24 hours old.
Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion : Test substance is considered to have moderate acute toxicity.
Reliability : (2) valid with restrictions
Performed using a proposed standardized test.
Flag : Critical study for SIDS endpoint
04.04.2006 (1) (2)

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)

Unit	:	mg/l
EC50	:	= 56 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C7 alcohol with a Kow of 2.24. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion	:	Based on the calculated Kow value, the C7 alcohol is expected to have an acute 48-hour EC50 of 56 mg/L and a Chronic Value of 3.2 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.04.2006 (4)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 35 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	other TS
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C7 alcohol with a Kow of 2.24. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion	:	Based on the calculated Kow value, the C7 alcohol is expected to have an

acute 96-hour EC50 of 35 mg/L and a Chronic Value of 4.1 mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

04.04.2006 (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species : other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint : other: LC50
Exposure period : 30 day(s)
Unit : mg/l
ChV : = 6.9 calculated
Method : other: calculated
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C7 alcohol with a Kow of 2.24.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched

Conclusion : Based on the calculated Kow value, the C7 alcohol is expected to have a 30-day Chronic Value of 6.9 mg/L

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

04.04.2006 (3)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : mortality
Exposure period : 16 day(s)
Unit : mg/l
EC50 : = 3.2 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database

of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C7 alcohol with a Kow of 2.24.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion : Based on the calculated Kow value, the C7 alcohol is expected yo have a 16-day EC50 of 3.2 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
04.04.2006 (3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type :
Species : other: Earthworm
Endpoint : mortality
Exposure period : 14 day(s)
Unit : mg/kg soil dw
LC50 : = 603 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C7 alcohol with a Kow of 2.24.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion : Based on the calculated Kow value, the C7 alcohol is expected to have a 14-day EC50 of 603 mg/kg soil.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
04.04.2006 (3)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 3900 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: None
Doses	:	
Method	:	other
Year	:	1979
GLP	:	no data
Test substance	:	
Remark	:	All animals in the 6.81 and 10.00 g/kg groups died. Two of the five animals in the 4.64 g/kg group died and 1 animal each in the 1.00, 2.15, and 3.15 g/kg groups died. No animals in the 1.47 g/kg group died. Except for one animal in the 2.15 g/kg group, all animals that died did so within three days of dosing. Signs of toxicity observed included respiratory rate decreases, fecal staining, decreased motor activity and hypothermia. Route of administration: Oral Intubation Frequency of Treatment: Single Exposure Dose/Concentration Levels: 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg Control group and Treatment: None
Result	:	LD50 = 3.9 g/kg
Test condition	:	Animals were fasted for approximately 18 hours prior to dosing. The undiluted test material was administered by oral intubation at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg (5 rats/dose). Animals were observed for signs of toxicity at 1, 2, and 4 hours after dosing and daily thereafter for fourteen days.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion	:	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute oral toxicity.
Reliability	:	(2) valid with restrictions Only one sex tested

04.04.2006 (5)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 152 ppm
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1979
GLP	:	no data
Test substance	:	

Remark	:	No abnormalities were noted in the control or exposed rats during the exposure period. Upon removal from the chamber, dry rales (1/10) and excessive salivation (2/10) were observed in exposed rats. Necropsy examination revealed an increased incidence of lung discoloration in treated rats (6/10). Route of administration: Inhalation Frequency of Treatment: Single Dose/Concentration Levels: 0, 152 ppm
Result	:	LC50 > 152 ppm
Test condition	:	Animals (5/sex/dose) were held for a minimum equilibration period of 12 days. Animals were exposed to 152 ppm of the test material for six hours. To generate vapors, room air was drawn through the test material at a flow rate of 103 l/min. The resulting maximum attainable vapors were passed through a Kjeldahl trap and flask prior to entering the glass exposure chamber containing the test animals. Weight loss was determined following exposure and was taken to be equal to the amount of test material delivered during exposure. The weight loss was divided by the total volume of air passed through the chamber to give the nominal concentration. The animals were exposed in the same chamber. For each species, a control group was also sham-exposed to room air. The animals were observed for abnormalities prior to exposure, at 15-minute intervals during the first hour of exposure and then hourly for the remainder of exposure. Subsequent evaluations were made for a total of 14 days. After fourteen days, gross necropsy was performed.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion	:	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute inhalation toxicity in rats.
Reliability	:	(2) valid with restrictions Vapor concentration not analyzed
Flag	:	Critical study for SIDS endpoint

04.04.2006 (7)

Type	:	LC50
Value	:	> 152 ppm
Species	:	mouse
Strain	:	other: Swiss albino
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: NA
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1979
GLP	:	no data
Test substance	:	

Remark	:	No abnormalities were noted in the control or exposed mice during the exposure period. During the 14-day observation period, excessive salivation was observed in mice (4/10) and nasal discharge (2/10) occurred. Route of administration: Inhalation Frequency of Treatment: Single Dose/Concentration Levels: 0, 152 ppm
Result	:	LC50 > 152 ppm
Test condition	:	Animals (5/sex/dose) were held for a minimum equilibration period of 12 days. Animals were exposed to 152 ppm of the test material for six hours. To generate vapors, room air was drawn through the test material at a flow rate of 103 l/min. The resulting maximum attainable vapors were passed through a Kjeldahl trap and flask prior to entering the glass exposure chamber containing the test animals. Weight loss was determined following exposure and was taken to be equal to the amount of test material delivered during exposure. The weight loss was divided by the

total volume of air passed through the chamber to give the nominal concentration. The animals were exposed in the same chamber. For each species, a control group was also sham-exposed to room air. The animals were observed for abnormalities prior to exposure, at 15-minute intervals during the first hour of exposure and then hourly for the remainder of exposure. Subsequent evaluations were made for a total of 14 days. After fourteen days, gross necropsy was performed.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion : Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute inhalation toxicity in mice.
Reliability : (2) valid with restrictions
Vapor concentration not analyzed
Flag : Critical study for SIDS endpoint
04.04.2006 (7)

Type : LC50
Value : > 152 ppm
Species : guinea pig
Strain : Hartley
Sex : male/female
Number of animals : 10
Vehicle : other: NA
Doses :
Exposure time : 6 hour(s)
Method : other
Year : 1979
GLP : no data
Test substance :

Remark : No abnormalities were noted in the control or exposed guinea pigs during the exposure period. Necropsy examination revealed an increased incidence of lung discoloration in treated guinea pigs (8/10).
Route of administration: Inhalation
Frequency of Treatment: Single
Dose/Concentration Levels: 0, 152 ppm
Result : LC50 > 152 ppm
Test condition : Animals (5/sex/dose) were held for a minimum equilibration period of 12 days. Animals were exposed to 152 ppm of the test material for six hours. To generate vapors, room air was drawn through the test material at a flow rate of 103 l/min. The resulting maximum attainable vapors were passed through a Kjeldahl trap and flask prior to entering the glass exposure chamber containing the test animals. Weight loss was determined following exposure and was taken to be equal to the amount of test material delivered during exposure. The weight loss was divided by the total volume of air passed through the chamber to give the nominal concentration. All three species were exposed in the same chamber. For each species, a control group was also sham-exposed to room air. The animals were observed for abnormalities prior to exposure, at 15-minute intervals during the first hour of exposure and then hourly for the remainder of exposure. Subsequent evaluations were made for a total of 14 days. After fourteen days, gross necropsy was performed.
Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion : Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute inhalation toxicity in guinea pigs.
Reliability : (2) valid with restrictions
Vapor concentration not analyzed
Flag : Critical study for SIDS endpoint
04.04.2006 (7)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: None
Doses	:	
Method	:	other
Year	:	1979
GLP	:	no data
Test substance	:	
Remark	:	Route of administration: Dermal Frequency of Treatment: Single Dose Dose/Concentration Levels: 50, 200, 794 and 3,160 mg/kg Control group and Treatment: None There were no deaths at any dose level in either sex. All animals at the 50 mg/kg level exhibited very slight erythema and no edema. Well-defined erythema without edema was observed in animals at 200 and 794 mg/kg dose levels. At the 3160 mg/kg dose level one animal exhibited moderate to severe erythema and three animals exhibited areas of necrosis. Necropsy examinations did not reveal any significant abnormalities. Dark red foci were observed in the lungs of males (50mg/kg) and females (3,160 mg/kg), however this effect was not dose-related. Dark red foci of the adrenals were observed in males and females at 200, 794, and 3,160 mg/kg.
Result	:	LD50 > 3160 mg/kg of body weight.
Test condition	:	Doses of 50, 200, 794 and 3160 mg/kg were administered to sixteen rabbits (two/sex/dose level). The undiluted test material was applied to intact skin and the animal was then wrapped in an impervious plastic sleeve. Following approximately 24 hours of exposure, the wrappings were removed and the test site was wiped free of excess test material. After 30 minutes, dermal observations were made. Observations were recorded at 1, 2 and 4 hours after dosing and daily thereafter for 14 days.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion	:	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute dermal toxicity in rabbits.
Reliability	:	(2) valid with restrictions GLP not specified
Flag	:	Critical study for SIDS endpoint

04.04.2006 (6)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	3.2 other: g/kg
Exposure	:	Occlusive
Exposure time	:	24 hour(s)
Number of animals	:	4
Vehicle	:	
PDII	:	
Result	:	

Classification	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	
Result	:	Group mean scores at 24, 48, and 72 hours were 1.5, 2.0, 4.0 for erythema and 2.5, 2.5, and 2.5 for edema. Dermal reactions were severe in all animals from Day 7 to 14.
Test condition	:	New Zealand White rabbits, at least 8 weeks old were acclimated to laboratory conditions for at least one week prior to use in the test. Animals were housed in accordance with AAALAC standards. Immediately prior to dosing, the fur was clipped from the abdomen of the animals. Abrasions were made in the skin of all animals. The abrasions scratched the stratum corneum, but did not reach the derma or produce bleeding. One group of 4 rabbits (2 males, 2 females) was dosed at 3.16 g/kg. The test material was applied once dermally to the prepared site under gauze patches. The patches were secured with adhesive tape and the trunks wrapped with impervious material. The test material was kept in contact with the skin for 24 hours, at which time the wrappings were removed. The exposure site was washed with water or corn oil to remove excess material. Dermal observations were scored at 24 hours, and 3, 7, 10 and 14 days after dosing by the Draize scoring system. The rabbits were observed 2 and 4 hours post dosing, and daily for 14 days for signs of toxicity, pharmacological effects and mortality. Body weights were recorded pretest and in the survivors at 14 days.
Test substance	:	CAS No. 70914-20-4; Alcohols, C6-8 branched
Conclusion	:	Under the conditions of the study, Alcohols, C6-8 branched produced significant irritation to rabbit skin.
Flag	:	Critical study for SIDS endpoint

04.04.2006 (8)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	highly irritating
Classification	:	
Method	:	other: similar to OECD TG 405
Year	:	1979
GLP	:	
Test substance	:	
Result	:	Median Scores were: 24 hr - 24 72 hr - 28 7 days - 5 Conjunctival irritation generally cleared by 10 days.

The maximum total Draize score observed was 51. Group mean scores at 24, 48, and 72 hours for the various indices were: 1.5, 1.5, 1.33 for conjunctival redness; 2.17, 2.5, 2 for chemosis; 1.0, 0.83, 0.83 for iridial irritation; 1.33, 1.5, 1.17 for corneal opacity.

Test condition : A single application of 0.1 ml of undiluted alcohol was made into the conjunctival sac of the left eye of each rabbit. The untreated eye served as the control. The treated eye was held closed for 1 second, and eyes were not washed.

Observations for irritancy and possible systemic toxicity were made at 1, 4, and 24 hours and at 2, 3, 4, and 7 days. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.04.2006 (9)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type : Sub-acute
Species : rat
Sex : male
Strain : Wistar
Route of admin. : gavage
Exposure period : 14 d
Frequency of treatm. : daily
Post exposure period : none
Doses : 130 mg/kg/bw/day (1 mM/kg bw)
Control group : yes, concurrent vehicle
NOAEL : >= 130 - mg/kg bw
Method : other: screening study
Year : 1984
GLP :
Test substance :

Remark : Comparative screening study to investigate selectively the effect on testis and liver morphology and function.

Result : Iso-octanol did not impair body weight and had no effect on relative liver and testis weight. Neither clinical pathology parameter nor peroxisome associated enzymes were affected. Liver histology differed not from the concurrent control group.

Test condition : Test species:
Male rats (Wistar derived) (breeder: ICI Alderley Park, UK)
10 per control group, 5 per dose group

Housing and diet:
1 week acclimatization
Caging: single, stainless-steel, screen-bottom cages
food and water ad libitum

Administration:
The substance was dissolved in polyethylene glycol 300 and 5 male rats received a dose level of 168 mg/kg bw (equivalent

to 1 mmol/kg bw) daily by gavage for 14 consecutive days. Application volume was 10 ml/kg bw. 10 control rats received the solvent in parallel.

Examinations:
Body weights were determined. The animals were killed by halothane overdose and blood samples for clinical pathology were taken. The liver was weighed and samples for light and electron microscopy, morphometric analysis were investigated. Remaining liver was processed for investigation of catalase and CN-insensitive palmitoyl CoA oxidation.

Test substance : Analogue substance: iso-octanol (CAS not specified).
Conclusion : Under the conditions of the study, iso-octanol has a low order of repeated dose toxicity to male rats for the endpoints studied. The NOAEL was the limit dose of 130 mg/kg.
Reliability : (2) valid with restrictions
Screening study with limited examinations but scientifically valid and well documented. From peer reviewed literature.
Flag : Critical study for SIDS endpoint
04.04.2006 (23)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Chromosomal aberration test
System of testing : Assay using Chinese hamster ovary (CHO) cells
Test concentration : 3.13, 10, 31.3, 100 and 313 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : EPA OPPTS 870.5375
Year : 2005
GLP : yes
Test substance :

Method : The study consisted of two phases: an initial chromosomal aberration assay with a 19 hour harvest time, and a repeat assay with both 19 and 43 hour cell harvest times. For the initial assay the test substance was mixed in acetone and tested at concentrations of 3.13, 10, 31.3, 100 and 313 ug/ml with metabolic activation (+S9) and 6.25, 20, 62.5, 200, and 625 ug/ml without metabolic activation (-S9). These concentrations were selected based on a previous toxicity pretest. The same concentrations were tested in the 19-hour and 43-hour repeat assays.

The CHO cells were cultured in McCoy's 5A Medium containing 10% fetal bovine serum and 2 mM L-glutamine and 1% penicillin/streptomycin at 37±2oC, in 4-6% CO2 in air. Two sets of duplicate cultures were prepared; one set was treated with the test substance with activation (+S9) and the other was treated with the test substance without activation (-S9). Each flask received a 50 mL sample of the test substance mixture, positive control mixture (N-Methyl-N'-Nitro-N-Nitrosoguanidine, MNNG, or 9,10-Dimethyl-1,2-benzanthracene (same as 7,12 Dimethylbenz[a]anthracene), DMBA), or vehicle (acetone). Flasks were treated for 3 hours for both +S9 and -S9 in the initial assay. In the repeat assay, flasks were treated for 3 hours for the +S9 and for 19 hours for -S9. The cultures were incubated to their respective harvest times (19 or 43 hours). A spindle inhibitor was added to the flasks approximately 1-3 hours prior to harvest to arrest the cells in c-metaphase. The cells were harvested and slides prepared to evaluate chromosomes. The positive control materials were evaluated for chromosomal aberrations at the 19 hour harvests only.

Based on confluency data generated during the study, 3.13, 31.3 and 313 mg/mL were selected as the doses to be evaluated for chromosomal aberrations with metabolic activation for both the initial and repeat assays. The doses picked to be evaluated for chromosomal aberrations without metabolic activation were also based on confluency data. The doses evaluated for the initial assay without metabolic activation (-S9) were 6.25, 62.5 200 and 625 mg/mL. The doses evaluated for the 19 hour repeat assay without metabolic activation (-S9) were 6.25, 62.5 200 and 625 mg/mL. The doses evaluated for the 43 hr repeat assay without metabolic activation (-S9) were 6.25, 62.5 and 200 mg/mL.

Result : There were no statistically significant differences or dose-related trends noted at any dose level in the initial or the repeat assay.

The positive control substances, DMBA and MNNG, produced statistically significant increases in the percentage of aberrant cells when tested with activation (DMBA) or without activation (MNNG) when compared to the vehicle control. Thus, the test system responded in an appropriate manner to these known clastogens. The vehicle control used in this study (acetone) also performed in a manner consistent with the criteria established for a valid assay.

Test substance : CAS No. 70914-20-4; Alcohols, C6-8 branched

Conclusion : Under the conditions of this study, the test substance did not induce chromosomal aberrations in CHO cells in the initial assay or the repeat assay.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

04.04.2006 (11)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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(21) Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(22) Meylan, W., Howard, P.H. and R.S. Boethling. (1992). Molecular Topolgy/Fragment Contribution Method for Predicting Soil Sorption Coefficients. Environ. Sci. Technol. 26:1560-7.

(23) Rhodes C, Soames T, Stonard MD, Simpson MG, Vernall AJ and Elcombe CR (1984). The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols, Tox. Lett. 21, 103-109

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 68526-85-2
CAS No.	:	68526-85-2
EINECS Name	:	Alcohols, C9-11-iso-, C10-rich
EC No.	:	271-234-0
TSCA Name	:	Alcohols, C9-11-iso-, C10-rich
IUPAC Name	:	Alcohols, C9-C11, branched

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.09.2004

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.09.2004
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	06.04.2006
Revision date	:	
Date of last update	:	06.04.2006
Number of pages	:	39
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C10H22O
Molecular weight : 160.26
Petrol class :

Flag : Critical study for SIDS endpoint
03.02.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 85566-14-9
IUPAC Name: Alcohols, C7-11-branched and linear
R Length (C number): C7 to C11
Structure of R: Linear
Category Member: No (analogue substance used for supporting information)

CAS RN: 68526-85-2
IUPAC Name: Alcohols C9-C11-iso, C10 rich
R Length (C number): C7
Structure of R: Branched, primarily methyl branched (isomeric structures)
Category Member: Yes

06.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Exxal(r) 10

15.03.2004

IDA

09.03.2004

Isodecanol

09.03.2004

Isodecyl alcohol

09.03.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	68526-85-2
EC-No	:	271-234-0
EINECS-Name	:	Alcohols, C9-11-iso-, C10-rich
Molecular formula	:	C9H20O2
Value	:	= 99.6 % w/w

Remark : Commercial product typically consists of trimethyl-1-heptanols and

dimethyl-1-octanols.
06.01.2005

1.4 ADDITIVES

Purity type	:	typical for marketed substance
CAS-No	:	
EC-No	:	
EINECS-Name	:	
Molecular formula	:	
Value	:	
Function of additive	:	
Remark	:	No additives present.

11.10.2005

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis
Remark	:	Primarily used as a chemical intermediate in the production of plasticizers.

06.01.2005

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -40 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: ASTM D97
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (1) (15)

2.2 BOILING POINT

Value	:	= 216 - 226 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (15)

2.3 DENSITY

Type	:	density
Value	:	.837 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	1998
GLP	:	yes
Test substance	:	
Method	:	The density was measured by taking the weight of 10 mls of the test substance at 20 deg C.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (9)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .018 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no data
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (21)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 4.2 - 4.3 at 30 °C
pH value	:	
Method	:	OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1998
GLP	:	yes
Test substance	:	
Remark	:	Test Type: N-Octanol/Water Partition Coefficient (HPLC method)
Result	:	The test substance eluted as several groups. The two major components C9, C10 alcohols had Log Pow values of 4.2 and 4.3, respectively. The retention time for the 2 major components were 8.37, and 8.74 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Test condition	:	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.

Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (12)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 75 mg/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Slow stir
Year	:	1998
GLP	:	no data
Test substance	:	

Method :

Slow-stir water solubility vessels consisted of glass aspirator bottles with capacities of 4 to 12 L. The spigot at the bottom of the vessel was fitted with short length of Tefzel tubing and a #13 glass stopper. The bottle was rinsed with a mixture of 1:1 methylene chloride : acetone followed by 2,2,4-trimethyl pentane. The bottle was then air dried in a laboratory fume hood and rinsed three times with dilution water.

A glass stir bar was added to the bottle and then the bottle was filled with the appropriate amount of water. The test substance was added to the bottle at a loading of 100 mg/L and the solution stirred quiescently with little or no visible vortex on a magnetic stir-plate.

Mixing was stopped one hour prior to sampling. Samples were removed through the outlet at the bottom of the vessel. To avoid losses and to prevent contamination, the samples were analyzed immediately by either GC-MSD or GC-FID. Samples were taken on Days 1, 3, 7, and 21.

Remark	:	Measured value obtained in conjunction with Fish Acute Toxicity Test.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (18)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 97 °C
Type	:	closed cup
Method	:	other: PMCC ASTM D93
Year	:	2003
GLP	:	no data
Test substance	:	

Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions

Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

06.04.2006 (15)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.89 to 17.52 at 25°C
Method	:	other: calculated
Year	:	2005
GLP	:	no data
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (17)

2.13 VISCOSITY

Value	:	= 21 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

06.04.2006 (15)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (14)

Type :
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000212981 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance :

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
6.0	21.30 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition	:	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance. This robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (22)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other: Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.
Result	:	Hydolysis as a Function of Molecular Structure Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis. Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982). References: Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press,

Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.

Flag : Critical study for SIDS endpoint

20.03.2006 (13)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 160.26 g/mol
Water solubility = 75 mg/L
Vapour pressure = 1.8 Pa
log Kow = 4.2
Melting point = -40 deg C

Degradation half-lives:

Air - 6.0 hrs
Water - 240 hrs
Soil - 1440 hrs
Sediment - 14400 hrs

This model was run assuming 100% discharge to water.

Result : Air - 0.2%
Water - 66.0%
Soil - 0.03%

Sediment - 33.8%

Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
25.10.2005 (20)

Type :
Media : other: air - biota - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level I
Year : 2003

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 160.26 g/mol
Water solubility = 75 mg/L
Vapour pressure = 1.8 Pa
log Kow = 4.2
Melting point = -40 deg C

Remark : Results were calculated using measured value for log Kow
Result : Air - 4.8%
Water - 6.2%
Soil - 87.0%
Sediment - 1.9%
Suspended Sed - 0.06%
Biota - <0.01%
Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
25.10.2005 (20)

Type : volatility
Media : water - air
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculation
Year : 2005

Method : Henry's Law Constants (HLC) are based on vapor pressure and water solubility values, and molecular weights. HLC values were calculated using equations found in Mackay, 2003.

Vapor pressure = 1.8 Pa
Water solubility = 75 mg/l
Molecular mass = 160.26 g/mol

Result : HLC (at 25 deg C) = 3.80 Pa-m3/mole
Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of (2) because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
26.10.2005 (20)

3.3.2 DISTRIBUTION

Media : other: Koc
Method : other (calculation)
Year : 2005

Method : The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980).

PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems.

Result : Koc = 67.19
log Koc = 1.827
Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
03.11.2005 (19) (23)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Contact time :
Degradation : = 71.1 (±) % after 28 day(s)
Result : other
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1997
GLP : yes
Test substance :

Remark : Test Type: Manometric Respirometry Test
Exposure Period: 28 days
Result : Test material is rapidly biodegradable. Half-life was reached by day 11. By day 28, 71.1% degradation of the test material was observed. 10% biodegradation was achieved on day 4 and 60% biodegradation was achieved on day 17.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were

noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	74.0, 72.6, 66.5	71.1
Na Benzoate	91.3, 81.3	86.3

* replicate data

Test condition : Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich

Conclusion : Test substance is considered rapidly biodegradable. Although the test substance (a complex and poorly water soluble material) achieived a ready extent of biodegradability, it did not achieve this extent within a 10-day window.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.04.2006 (10)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : Oncorhynchus mykiss (Fish, fresh water)

Exposure period : 16 day(s) at 14.6 °C

Concentration :

BCF : 15

Elimination :

Method : OECD Guide-line 305

Year : 1998

GLP : yes

Test substance :

Remark :

No difference in mortality or growth was observed between the treatments and the control after 16 days of exposure, or at the end of the study (26 days).
Duration: 16 days uptake, 10 days depuration

The duration of the uptake phase was shorter than the guideline recommended duration of 28 days. The duration of the uptake phase was determined based on the concentration of the test substance reaching a steady state in the tissue of the fish. Samples of the fish were analyzed at regular intervals. To determine the concentration of the test substance in

the fish tissue, under steady-state conditions, one-tail T-tests for the comparison of the means at the sampling times were performed.

Result : Calculated Bioconcentration Factor (BCF):
0.75 mg/L = 14.8
0.15 mg/L = 15.5
Mean BCF for the study = 15.2

Test condition : A 100 mg/L stock solution was prepared by adding the appropriate amount of the test substance to 18 liters of dilution water. The stock solution was mixed for 24 hours prior to its use in the test. It was then pumped from the mixing vessel via a glass tube, silicon tubing and varistaltic pump and delivered to the test chambers via a 2 liter proportional diluter. Two concentrations were prepared for the test, 0.75 mg/L and 0.15 mg/L. A dilution water control was also prepared. A new stock solution was prepared in this manner every 4 days and mixed for 24 hours prior to use in the test.
One test chamber was prepared for each treatment and the control. At the start of the test each test chamber contained 45 fish. Fish were observed daily for mortality and/or abnormal behavior or appearance. Water and fish samples were removed periodically during both the uptake and depuration phases of the study. Samples were analyzed by gas chromatography.
Mean measured concentrations of the test substance in water :
0.75 mg/L = 0.91 mg/L (s.d.= 0.15)
0.15 mg/L = 0.16 mg/L (s.d.= 0.02)
The test substance was not detected in the control during the study or in either treatment during the depuration phase.
Mean measured concentrations of the test substance in fish tissue:
0.75 mg/L = 13.8mg/kg
0.15 mg/L = 2.5 mg/kg
Fish samples were also removed at the beginning and end of the uptake phase and analyzed for lipid content. The mean percent lipid content was 3.53%.

Test temperature was 14.6 Deg C., Lighting was 16 hours light : 8 hours dark with 438 to 612 Lux during full daylight periods.

Dissolved Oxygen ranged from 8.7 to 9.3 mg/L. The pH was ranged from 7.1 to 7.3 during the study. Fish were fed at a rate of 2% of their bodyweight per day during the study.

Fish Mean Weight was approximately = 0.367g at the start of the test. Test Loading = 0.47 g of fish/L.

The following data represent the measurements of the test chemical in fish tissue. Units are in µg of test chemical per gram of fish. The Non Detect (ND) level was 0.2 µg/g, which corresponds to 0.67 µg/g for a 0.3 g fish and 0.14 µg/g for a 1.4 g fish mass.

Fish Tissue Analysis

	Uptake Phase					
	Day 1	Day 2	Day 4	Day 10	Day 16	
	ND	ND	ND	ND	ND	
Control	ND	ND	ND	ND	ND	
	ND	ND	ND	ND	ND	
	1.1	NS	1.2	2.7	1.5	
0.15mg/l	1.0	1.2	1.1	2.3	1.8	
	mean	1.1	1.2	1.2	2.5	1.7
	5.8	5.9	7.4	19	8.2	
0.75mg/l	7.2	2.8	8.6	13	15	

	mean	6.5	4.4	8.0	16.0	11.6

		Depuration Phase		
		Day 0	Day 1	Day 4
Control		ND	ND	ND
		ND	ND	ND
		ND	ND	ND
0.15mg/l		0.35	ND	ND
		0.57	ND	ND
		0.31		ND
	mean	0.41	ND	ND
0.75mg/l		2.0	0.40	ND
		2.1	0.17	ND
		4.2	0.30	ND
	mean	2.8	0.29	ND

Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion : Low potential to bioaccumulate. Value based on wet weight data.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.04.2006 (11)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 3.1 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1995
GLP	:	yes
Test substance	:	
Method	:	Probit procedure of SAS (Finney, 1971)
Result	:	LC50 = 3.1mg/L (CI 2.4 to 4.0), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-FID LL50 = 3.0 mg/L (Could not calculate CI), based upon nominal loading levels. Nominal Conc. Measured Conc. % Mortality @ 96 hr. Control Below detection 7 1.2 mg/L 1.2 mg/L 13 2.5 mg/L 2.4 mg/L 13 5 mg/L 5.2 mg/L 100 10 mg/L 9.9 mg/L 100 20 mg/L 19.5 mg/L 100 Dissolved oxygen levels dropped below 60% (57%)of saturation in the 2.4 mg/L treatment on Days 3 and 4 of the test. Since only 13% mortality occurred at this level, and the solutions were renewed daily, this drop in DO did not affect the outcome of the study.
Test condition	:	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19.5L of dilution water in a 20L glass carboy. The carboys were covered with an opaque covering to prevent photochemical degradation of the soluble components. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution. Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 569 to 572 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.9 mg/L and from 5.7 to 7.6 mg/L in "old" solutions prior to renewals. The pH was ranged from 7.0 to 8.5 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.185g. Mean Total length = 3.0cm, Test Loading = 0.21 g of fish/L.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Test substance is considered to have moderate acute toxicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (9)

Type	:	
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 3.1 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C10 alcohol with a Kow of 3.68. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Based on the calculated Kow value, the C10 alcohol is expected to have an acute 96-hour LC50 of 3.1 mg/L and a Chronic Value of 0.5 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 6.2 measured/nominal
Limit Test	:	no
Analytical monitoring	:	no
Method	:	other: Daphnid Acute Toxicity Test
Year	:	1982
GLP	:	no data
Test substance	:	other TS
Method	:	Methods for acute toxicity tests with fish, macroinvertebrates and amphibians (EPA-660/3-75-009) Moving average angle method.
Result	:	48-hour EC50 = 6.2 mg/L (95% CI 5.3-7.6 mg/L), based upon nominal concentrations.
Test condition	:	Individual treatments were prepared by adding the appropriate amount of the test substance to 1000 ml of dilution water and mixing vigorously on a magnetic stirrer for 4 hours. Four hundred and fifty milliliters of this test solution were divided into three replicate beakers, each containing 150 ml. A set of control beakers containing the same dilution water and maintained under the same conditions was also prepared.

Fifteen daphnids were exposed to each test concentration (5 per replicate). Daphnids were <24 hours old and were impartially distributed to the test chambers. Mortalities were recorded at 24 and 48 hours after initiation of the exposures. Biological observations were also made at this time.

Test temperature was 21-23 Deg C., Dissolved oxygen ranged from 7.7 to 8.4 mg/L during the study. The pH was ranged from 8.1 to 8.7 during the study.

Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion : Test substance is considered to have moderate acute toxicity.
Reliability : (2) valid with restrictions
Study followed acceptable study guidelines and was well documented. Analytical verification of test concentrations not test substance specific.
Flag : Critical study for SIDS endpoint
06.04.2006 (4)

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 3.7 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C10 alcohol with a Kow of 3.68.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion : Based on the calculated Kow value, the C10 alcohol is expected to have an acute 48-hour EC50 of 3.7 mg/L and a Chronic Value of 0.4 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
06.04.2006 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: Pseudokirchneriella subcapitata
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 2.6 calculated
ChV : = .68 calculated
Method : other: ECOSAR Computer Model

Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C10 alcohol with a Kow of 3.68.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Based on the calculated Kow value, the C10 alcohol is expected to have an acute 96-hour EC50 of 2.6 mg/L and a Chronic Value of 0.68 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= .492 calculated
Method	:	other: calculated
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C10 alcohol with a Kow of 3.68.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Based on the calculated Kow value, the C10 alcohol is expected to have a 30-day Chronic Value of 0.52 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia sp. (Crustacea)
Endpoint	:	mortality

Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= .4 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	no
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C10 alcohol with a Kow of 3.68.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Based on the calculated Kow value, the C10 alcohol is expected yo have a 16-day EC50 of 0.40 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: Earthworm
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/kg soil dw
LC50	:	= 295.8 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C10 alcohol with a Kow of 3.68.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Based on the calculated Kow value, the C10 alcohol is expected to have a 16-day EC50 of 295.8 mg/kg soil.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data

are calculated and not measured.

Flag : Critical study for SIDS endpoint
06.04.2006 (3)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 4626 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: corn oil
Doses	:	26, 82, 260, 820, 2600, 8200 mg/kg bw
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	5/5 animals died within the first four hours following exposure to 8200 mg/kg. Animals in all other dose groups survived until the end of the study. At the one and four-hour intervals, animals in the 260 and 820 mg/kg dose groups were inactive and displayed labored respiration, ataxia, and sprawling of the limbs. At the 24-hour interval, animals had oily fur. After approximately 48-hours after dosing, most animals in these groups returned to normal appearance and behavior. At the 2600 mg/kg dose level, animals exhibited similar symptoms as above but also showed lacrimation and depressed righting and placement reflexes. Animals in this dose group also returned to normal appearance and behavior after 24 hours. At the highest dose, animals initially exhibited labored respiration, ataxia, and sprawling of the limbs, which was followed by a comatose state and death within 4 hours of exposure. The surviving animals at the five lower dose levels (26, 82, 260, 820, 2600 mg/kg) had weight gain that was within the normal range. Gross autopsies performed on animals that died (5/5 in 8200 mg/kg group) revealed congested lungs, kidneys, and adrenals, and dark-appearing spleens. No abnormalities were observed in the surviving animals at necropsy. Therefore, a histopathologic analysis was not performed. Route of administration: Oral gavage Frequency of Treatment: Single Treatment Dose/Concentration Levels: 0.1, 1.0, 10.0, 30.0% volume/volume emulsion in corn oil (Equivalent to 26, 82, 260, 820, 2600, 8200 mg/kg) Control group and Treatment: For comparison, untreated animals were necropsied at the end of the study.
Result	:	LD50 = 4626 mg/kg
Test condition	:	Prior to dosage, food was withheld from the animals for three to four hours. The animals were observed for gross effects and mortality at one, four, and twenty-four hours, and once daily thereafter up until seven days. Gross necropsies were performed at the end of the observation period and samples of liver, kidney, brain, and blood were taken from untreated control animals and from all surviving animals at the 820 and 2600 mg/kg dose levels.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Under the conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of toxicity.
Reliability	:	(2) valid with restrictions Pre-GLP

Flag	:	Critical study for SIDS endpoint
06.04.2006		(5)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 95 ppm
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	10
Vehicle	:	other: not applicable
Doses	:	95 ppm
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	other TS: decyl alcohol (CAS No. 68526-85-2)
Remark	:	There were no deaths during the exposure, or during the 24-hour post-exposure period. Slight to moderate local irritation involving the mucous membranes of the eyes, nose, throat, and respiratory passages was seen, but quickly returned to normal at termination of exposure.
Result	:	LC50 > 95 ppm (approximately 0.6 mg/l)
Test condition	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 24-hour post-exposure observation period. Feed and water were freely available during the post-exposure holding period. Nearly saturated atmospheres were generated by fritted-disk bubblers containing a measured amount of the test substance through which all air entering the chambers was passed. Chamber concentrations were not determined. The nominal concentration was determined by the net loss of the test substance from the bubblers and the total airflow. After exposure, the animals were returned to their cages and observed for 24 hours.
Conclusion	:	Under the conditions of this study, decyl alcohol has a low order of acute inhalation toxicity in rats.
Reliability	:	(2) valid with restrictions Pre-GLP, vapor concentration not analyzed. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint
06.04.2006		(5) (26)

Type	:	LC50
Value	:	> 95 ppm
Species	:	mouse
Strain	:	other: Swiss albino
Sex	:	male
Number of animals	:	10
Vehicle	:	other: not applicable
Doses	:	95 ppm
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	other TS: decyl alcohol (CAS No. 68526-85-2)
Remark	:	There were no deaths during the exposure, or during the 24-hour post-exposure period. Slight to moderate local irritation involving the mucous membranes of the eyes, nose, throat, and respiratory passages was seen, but quickly returned to normal at termination of exposure.
Result	:	LC50 > 95 ppm (approximately 0.6 mg/l)

Test condition	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 24-hour post-exposure observation period. Feed and water were freely available during the post-exposure holding period. Nearly saturated atmospheres were generated by fritted-disk bubblers containing a measured amount of the test substance through which all air entering the chambers was passed. Chamber concentrations were not determined. The nominal concentration was determined by the net loss of the test substance from the bubblers and the total airflow. After exposure, the animals were returned to their cages and observed for 24 hours.
Conclusion	:	Under the conditions of this study, decyl alcohol has a low order of acute inhalation toxicity in mice.
Reliability	:	(2) valid with restrictions Pre-GLP, vapor concentration not analyzed.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (5) (26)

Type	:	LC50
Value	:	> 95 ppm
Species	:	guinea pig
Strain	:	Hartley
Sex	:	male
Number of animals	:	10
Vehicle	:	other: not applicable
Doses	:	95 ppm
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	other TS: decyl alcohol (CAS No. 68526-85-2)
Remark	:	There were no deaths during the exposure, or during the 24-hour post-exposure period. Slight to moderate local irritation involving the mucous membranes of the eyes, nose, throat, and respiratory passages was seen, but quickly returned to normal at termination of exposure.
Result	:	LC50 > 95 ppm (approximately 0.6 mg/l)
Test condition	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 24-hour post-exposure observation period. Feed and water were freely available during the post-exposure holding period. Nearly saturated atmospheres were generated by fritted-disk bubblers containing a measured amount of the test substance through which all air entering the chambers was passed. Chamber concentrations were not determined. The nominal concentration was determined by the net loss of the test substance from the bubblers and the total airflow. After exposure, the animals were returned to their cages and observed for 24 hours.
Conclusion	:	Under the conditions of this study, decyl alcohol has a low order of acute inhalation toxicity in guinea pigs.
Reliability	:	(2) valid with restrictions Pre-GLP, vapor concentration not analyzed. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (5) (26)

Type	:	other: Upper Airway Sensory Irritation
Value	:	280 ppm
Species	:	mouse
Strain	:	Swiss Webster
Sex	:	male
Number of animals	:	8
Vehicle	:	other: not applicable
Doses	:	111, 168 ppm
Exposure time	:	30 minute(s)

Method	:	other: ASTM: E981-84
Year	:	1993
GLP	:	yes
Test substance	:	
Remark	:	The maximum vapor concentration that could be achieved under the conditions of this study was 168 ppm. There were no deaths during the exposure, or during the post-exposure period. No evidence of pulmonary (deep lung) irritation was observed. No animals in either group showed ocular abnormalities during or after the exposure. Value is estimated Route of Administration: Head-only inhalation, aerosol
Result	:	None of the respiratory rate decreases exceeded 50%, therefore an RD50 concentration could only be estimated. 111 ppm resulted in 32% decrease in breathing pattern 168 ppm resulted in 40% decrease in breathing pattern RD50 = 280 ppm (estimated)
Test condition	:	The upper airway sensory irritation potential was evaluated in male Swiss Webster mice. The test material was generated as a vapor by bubbling compressed air through the liquid test substance contained inside two gas-washing bottles (bubblers) connected in series. The test animals received head-only exposures for 30 minutes. Respiratory rates were monitored before, during and after exposure, to establish a baseline respiratory rate, and to evaluate the animals' sensory irritation response to the test atmosphere.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	The test substance produced breathing patterns characteristic of upper airway sensory irritation in all both groups of male mice exposed to aerosol atmospheres ranging from 111 to 168 ppm.
Reliability	:	(1) valid without restriction

06.04.2006 (8)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2600 - mg/kg bw
Species	:	rabbit
Strain	:	other: Albino
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: none
Doses	:	80, 260, 820, and 2600 mg/kg bw
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	
Remark	:	No deaths were observed during this study. Mild to moderate erythema and edema were observed in animals at the three lower dose levels. Marked erythema and edema were observed at the highest dose level. Edema in each animal subsided within 3 days. Erythema in animals at the high dose group diminished in intensity but did not subside completely during the observation period. Autopsies performed following sacrifice revealed no gross pathological findings in any animal. Therefore, a histopathologic analysis was not performed. Route of administration: Dermal Frequency of Treatment: Single Dose Dose/Concentration Levels: 80, 260, 820, and 2600 mg/kg
Result	:	The acute dermal LD50 is > 2600 mg/kg

Test condition	:	A single application of the test material was given to four groups (2/sex/dose) of four rabbits at doses of 80, 260, 820, and 2600 mg/kg. The material was applied under occlusive dressing to intact abdominal skin. Observations were recorded at one, four and 24 hours; and once daily thereafter for a total of 7 days. Samples of liver, kidney, brain and blood were taken from four untreated control albino rabbits and from each surviving animal at the 820 and 2600 mg/kg dose level.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Conclusion	:	Under conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of acute dermal toxicity in rats.
Reliability	:	(2) valid with restrictions (Pre-GLP). From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (5) (26)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	.5 undiluted
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	other: none
PDII	:	2.16
Result	:	moderately irritating
Classification	:	
Method	:	other: OECD TG 404; EEC Directive 84/449, section B4
Year	:	1992
GLP	:	yes
Test substance	:	
Remark	:	Mean scores at 24, 48, and 72 hours were 1.33, 1.33, and 1.83 for erythema and 0.33, 0.5 and 0.83 for edema, respectively. Six male (13 weeks old) New Zealand White rabbits were used.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. Approximately 24 hours prior to application of the test substance, the dorsal fur was shaved with an electric clipper. On Day 1 of the study, 0.5 ml of the test substance was applied to the skin of the animal and covered with a patch of surgical gauze, which was then covered by a semi-occlusive dressing. The dressing was removed four hours after the application and the skin was flushed with reverse osmosis water. The skin reaction was assessed according to the test guidelines at 45 minutes, 24, 48, and 72 hours and at 7 days after the removal of the dressing. No animal deaths were recorded prior to study termination.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (7)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	

Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	none
Result	:	irritating
Classification	:	
Method	:	other: similar to OECD TG 405
Year	:	1970
GLP	:	no
Test substance	:	
Remark	:	Mean scores at 24, 48, and 72 hours were 1.8, 1.5, 1.3 for conjunctival redness, 0.5, 0, 0 for chemosis, 0.67, 0.5, 0.33 for iridial irritation, and 0.5, 0.5 and 0.33 for corneal opacity, respectively. Group median Draize score = 28 (out of 110) The test substance produced significant conjunctival irritation in the eyes of rabbits which generally cleared by 7 days. Rated as a severe eye irritant due to corneal sloughing or pitting.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The contralateral eye served as the control. The eyes of each animal were examined 24, 48, and 72 hours, and 4, 7 and 10 days after administration. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale.
Test substance	:	CAS No. 68526-85-2; Alcohols, C9-C11-iso, C10 rich
Reliability	:	(2) valid with restrictions Pre-GLP. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (6) (26)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-acute
Species	:	rat
Sex	:	male
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	14 d
Frequency of treatm.	:	daily
Post exposure period	:	none
Doses	:	168 mg/kg/bw/day (1 mM/kg bw)
Control group	:	yes, concurrent vehicle
Method	:	other: screening study
Year	:	1983
GLP	:	no data
Test substance	:	
Remark	:	Comparative screening study to investigate selectively the effect on testis and liver morphology and function.

Result	:	Isodecanol did not impair body weight and had no effect on relative liver and testis weight. Neither clinical pathology parameter nor peroxisome associated enzymes were affected. Liver histology differed not from the concurrent control group.
Test condition	:	Test species: Male rats (Wistar derived) (breeder: ICI Alderley Park, UK) 10 per control group, 5 per dose group Housing and diet: 1 week acclimatization Caging: single, stainless-steel, screen-bottom cages food and water ad libitum Administration: The substance was dissolved in polyethylene glycol 300 and 5 male rats received a dose level of 168 mg/kg bw (equivalent to 1 mmol/kg bw) daily by gavage for 14 consecutive days. Application volume was 10 ml/kg bw. 10 control rats received the solvent in parallel. Examinations: Body weights were determined. The animals were killed by halothane overdose and blood samples for clinical pathology were taken. The liver was weighed and samples for light and electron microscopy, morphometric analysis were investigated. Remaining liver was processed for investigation of catalase and CN-insensitive palmitoyl CoA oxidation.
Test substance	:	Analogue substance: Iso-decanol (CAS No. 25339-17-7) (supplied by ICI plc, UK)
Reliability	:	(2) valid with restrictions Screening study with limited examinations but scientifically valid and well documented. From peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (24) (25)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Cytogenetic assay
System of testing	:	V79 Chinese hamster lung fibroblasts
Test concentration	:	5 - 20 µg/ml
Cycotoxic concentr.	:	20 µg/ml
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	1983
GLP	:	yes
Test substance	:	
Method	:	V79 Chinese hamster lung cells were exposed to isodecanol with/without metabolic activation. Following exposure, the cells were treated with colcemid to arrest cells in the metaphase. Cells were harvested and chromosome preparations were made. The preparations were stained with Giemsa and metaphase cells were analyzed for chromosomal aberrations. Cytotoxicity as depression of the mitotic index was previously examined and Ethylmethanesulonate and Cyclophosphamide were used as positive control substances.

		Each 100 well spread metaphases per treatment group were examined and two independent experiments were performed.
Test condition	:	Test system: V79 Chinese hamster lung fibroblasts Tests: a) without S-9 mix, fixation time 21 h after start of treatment, concentrations: 5, 10 and 20 µg/ml b) with S-9 mix, exposure 3 h, fixation time 18 h after start of treatment, concentrations: 5, 10 and 20 µg/ml c) with S-9 mix, exposure 3 h, fixation time 21 h after start of treatment, concentrations: 5, 10 and 20 µg/ml Solvent: Ethanol Positive control substances: Ethylmethanesulonate: 500 µg/ml Cyclophosphamide: 5 µg/ml
Test substance	:	Analogue substance: Isodecanol (CAS No. 25339-17-7), source: Riedel-de-Haen, Seelze, Germany, colorless liquid
Conclusion	:	Isodecanol induced no chromosomal aberrations in cultured mammalian V79 cells with/without metabolic activation.
Reliability	:	(1) valid without restriction GLP guideline study described in sufficient detail.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (16)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	
Strain	:	
Route of admin.	:	gavage
Exposure period	:	once
Doses	:	2.26-12.8 mg/kg (1/5 LD50)
Result	:	
Method	:	
Year	:	1987
GLP	:	
Test substance	:	
Method	:	Each 10 rats were investigated, 1 ml test article/rat was orally administered by gavage as a 40% suspension in water. Preparation of bone marrow 48 h after administration and microscopic analysis of 50 cells per animal. Number of cells investigated was too few to correspond to scientific and regulatory requirements. Original reference in Russian.
Result	:	3% of cells with aberration were observed, control group 0% of cells with aberrations.
Test substance	:	Analogue substance: Decylalcohol (CAS No. 25339-17-7)
Reliability	:	(2) valid with restrictions Documentation insufficient for assessment since reference is in a foreign language. However, reference is from a peer reviewed journal.

06.04.2006 (2)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 68526-86-3
CAS No.	:	68526-86-3
EINECS Name	:	Alcohols, C11-14-iso-, C13-rich
EC No.	:	271-235-6
TSCA Name	:	Alcohols, C11-14-iso-, C13-rich
IUPAC Name	:	Alcohols C11-C14 iso, C13 rich

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.09.2004

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	29.09.2004
Status	:	
Memo	:	Prepared for EMCC - US HPV
Printing date	:	06.04.2006
Revision date	:	
Date of last update	:	06.04.2006
Number of pages	:	42
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : see free text

Remark : The Alkyl Alcohols C6 to C13 Category is a family of saturated alcohols that are produced from olefins by the hydroformylation or "oxo" process. Hydroformylation is the reaction of an olefin with carbon monoxide and hydrogen to produce an aldehyde, and its subsequent hydrogenation to the alcohol.

The number of carbon atoms in the category members ranges from 6 to 13. Category members contain predominantly branched alkyl groups. Each substance consists of an isomeric mixture of saturated primary alcohols of high purity, and the following basic structure: CH3-R-CH2-OH, where R is a branched isomeric structure.

The justification for the Alkyl Alcohols C6 to C13 Category is that the members have:
· similar chemical structures,
· similar physico-chemical properties,
· comparable environmental fate,
· the same mode of action.

In general, aliphatic alcohol toxicity occurs by non-polar narcosis (Lipnick et al., 1985). The mode of action is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Metabolic pathways, through which alcohols are metabolized, are likely to include similar reactions for all category members and result in structurally similar metabolites (carboxylic acids).

The data demonstrate that the category is valid for a screening-level hazard assessment for the Category and its members. One can assess the untested endpoints by extrapolation between and among the category members.

20.03.2006

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :
Smiles Code :
Molecular formula : C13H28O
Molecular weight : 200.37
Petrol class :

Flag : Critical study for SIDS endpoint
11.01.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Remark : CAS Registry Number, Name, and General Structure for Members of the Alkyl Alcohols C6 to C13 Category and Analogue Substances:

CAS RN: 112-53-8
IUPAC Name: Dodecan-1-ol
R Length (C number): C12
Structure of R: Linear
Category Member: No (analogue substance used for supporting information)

CAS RN: 68526-86-3
IUPAC Name: Alcohols C11-C14-iso, C13 rich
R Length (C number): C10
Structure of R: Branched, primarily methyl branched (isomeric structures)
Category Member: Yes

06.04.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Exxal(r) 13

15.03.2004

Isotridecanol

09.03.2004

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	68526-86-3
EC-No	:	271-235-6
EINECS-Name	:	Alcohols, C11-14-iso-, C13-rich
Molecular formula	:	C13H28O
Value	:	= 99.8 % w/w

Remark : Major isomers are tetramethyl-1-decanol and dimethyl-1-undecanol.
11.10.2005

1.4 ADDITIVES

Purity type : typical for marketed substance

CAS-No	:	
EC-No	:	
EINECS-Name	:	
Molecular formula	:	
Value	:	
Function of additive	:	
Remark	:	No additives present.

11.10.2005

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis
Remark	:	Primarily used as a chemical intermediate in the production of plasticizers because of their low volatility. Also used as a surfactant raw material, as a lubricant intermediate, and as a solvent.

06.01.2005

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	< -40 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: ASTM D97
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (1) (16)

2.2 BOILING POINT

Value	:	= 250 - 270 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078/01
Year	:	2003
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (16)

2.3 DENSITY

Type	:	density
Value	:	.846 g/cm³ at 20 °C
Method	:	other: ASTM D4052/86 equivalent
Year	:	1998
GLP	:	no data
Test substance	:	
Method	:	The density was measured by taking the weight of 10 mls of the test substance at 20 deg C.
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (9)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .002 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no data
Test substance	:	
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (23)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 4.8 - 5.5 at 30 °C
pH value	:	
Method	:	OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1998
GLP	:	yes
Test substance	:	
Remark	:	Test Type: N-Octanol/Water Partition Coefficient (HPLC method)
Result	:	The test substance eluted as several groups. The four major components C10, C11, C12, C13 alcohols had Log Pow values of 4.8, 5.0, 5.1, and 5.5 respectively. The retention time for the 4 major components were 12.09, 13.72, 14.76, and 18.36 minutes. All values were measured using High Performance Liquid Chromatography (HPLC).
Test condition	:	The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4. Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3. The pH of the evaluated solutions was the same as the reference solution it was evaluated against. The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound

Solution. Only the peaks detected by refractive index (RI) were reported.

Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.04.2006 (7)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 5.8 mg/l at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: slow stir
Year : 1998
GLP : no data
Test substance :

Method : Slow-stir water solubility vessels consisted of glass aspirator bottles with capacities of 4 to 12 L. The spigot at the bottom of the vessel was fitted with short length of Tefzel tubing and a #13 glass stopper. The bottle was rinsed with a mixture of 1:1 methylene chloride : acetone followed by 2,2,4-trimethyl pentane. The bottle was then air dried in a laboratory fume hood and rinsed three times with dilution water.

A glass stir bar was added to the bottle and then the bottle was filled with the appropriate amount of water. The test substance was added to the bottle at a loading of 100 mg/L and the solution stirred quiescently with little or no visible vortex on a magnetic stir-plate.

Mixing was stopped one hour prior to sampling. Samples were removed through the outlet at the bottom of the vessel. To avoid losses and to prevent contamination, the samples were analyzed immediately by either GC-MSD or GC-FID. Samples were taken on Days 1, 3, 7, and 21.

Remark : Measured value obtained in conjunction with Fish Acute Toxicity Test.
Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.04.2006 (20)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 126 °C
Type : closed cup
Method : other: PMCC ASTM D93
Year : 2005
GLP : no data
Test substance :

Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich

Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

06.04.2006 (16)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Acid-base constant	:	= 15.935 at 25°C
Method	:	other: calculated
Year	:	2005
GLP	:	no data
Test substance	:	
Method	:	pKa calculation by SPARC 2003 using a Linux calculation engine.
Remark	:	SPARC On-line calculator can be accessed at http://ibmlc2.chem.uga.edu/sparc/index.cfm
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by SPARC. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (19)

2.13 VISCOSITY

Value	:	= 47 - at 20 °C
Result	:	
Method	:	other: ASTM D445
Year	:	2003
GLP	:	no data
Test substance	:	
Remark	:	Value measured in cSt
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable.

06.04.2006 (16)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Oxo Alcohols C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb UV light below 220 nm (Boethling and Mackay, 2000) and will not undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical

Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Alkyl Alcohols C6 to C13 Category members
Flag : Critical study for SIDS endpoint
03.04.2006 (15)

Type :
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000195991 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance :

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
6.5	19.60 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition	:	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E6 OH radicals/cm3
Test substance	:	CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability	:	(2) valid with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance. This robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (24)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other: Technical Discussion
Year	:	
GLP	:	
Test substance	:	
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Alcohols C6 to C13 Category to undergo hydrolysis.
Result	:	Hydolysis as a Function of Molecular Structure Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have the potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a leaving group renders a compound resistant to hydrolysis. Alkyl alcohols are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive (Harris, 1982). References: Gould, E.S. (1959). Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. Harris, J.C. (1982). "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. Neely, W.B. (1985). Hydrolysis. In: W.B. Neely and G.E. Blau, eds., Environmental Exposure from Chemicals. Vol. 1, pp. 157-173. CRC Press,

Boca Raton, FL, USA.

Conclusion : Hydrolysis will not contribute to the removal of Alkyl Alcohols from the environment.

Flag : Critical study for SIDS endpoint

20.03.2006 (14)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level III
Year : 2003

Method : The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 200.37 g/mol
Water solubility = 5.8 mg/L
Vapour pressure = 0.2 Pa
log Kow = 5.15
Melting point = -40 deg C

Degradation half-lives:

Air - 6.5 hrs
Water - 240 hrs
Soil - 1440 hrs
Sediment - 14400 hrs

This model was run assuming 100% discharge to water.

Result : Air - 0.08%
Water - 18.3%
Soil - 0.01%

Sediment - 81.6%

Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
25.10.2005 (22)

Type : fugacity model level I
Media : other: air - biota - sediment(s) - soil - water
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: Calculation according Mackay, Level I
Year : 2003

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 200.37 g/mol
Water solubility = 5.8 mg/L
Vapour pressure = 0.2 Pa
log Kow = 5.15
Melting point = -40 deg C

Remark : Results were calculated using measured value for log Kow.
Result : Air - 1.1%
Water - 0.8%
Soil - 96.0%
Sediment - 2.1%
Suspended Sed - 0.07%
Biota - 0.01%
Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
25.10.2005 (22)

Type : volatility
Media : water - air
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculation
Year : 2005

Method : Henry's Law Constants (HLC) are based on vapor pressure and water solubility values, and molecular weights. HLC values were calculated using equations found in Mackay, 2003.

Vapor pressure = 0.2 Pa
Water solubility = 5.8 mg/l
Molecular mass = 200.37 g/mol

Result : HLC (at 25 deg C) = 6.91 Pa-m3/mole
Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of (2) because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
26.10.2005 (22)

3.3.2 DISTRIBUTION

Media : other: Koc
Method : other (calculation)
Year : 2005

Method : The soil adsorption coefficient (Koc) was calculated by PCKOCWIN ver. 1.66, using equations developed by Lyman (1980).

PCKOCWIN is a subroutine of EPIWIN. EPIWIN is used and advocated by the USEPA for chemical property estimation. Koc provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems.

Result : Koc = 505.8
log Koc = 2.74
Test substance : CAS No. 68526-86-3; Alcohols, C11-C14-iso, C13 rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
26.10.2005 (21) (25)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Contact time :
Degradation : 60.6 (±) % after 28 day(s)
Result : other
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1999
GLP : yes
Test substance :

Remark : Test Type: Manometric Respirometry Test
Exposure Period: 28 days
Result : Test material is rapidly biodegradable. Half-life was reached on day 20. On day 28, 60.6% degradation of the test material was observed. 10% biodegradation was achieved on day 7.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	59.9, 62.7, 59.2	60.6
Na Benzoate	89.0, 87.4, 87.8	88.0

* replicate data

Test condition : Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 100 mg/L. Sodium benzoate (positive control) concentration was 50mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich

Conclusion : Test substance is considered rapidly biodegradable. Although the test substance (a complex and poorly water soluble material) achieived a ready extent of biodegradability, it did not achieve this extent within a 10-day window.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.04.2006 (12)

Type : aerobic

Inoculum : activated sludge, domestic

Contact time :

Degradation : = 58 (±) % after 28 day(s)

Result : other: not readily biodegradable

Deg. product :

Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"

Year : 1998

GLP : yes

Test substance :

Remark : Test Type: Manometric Respirometry Test
Exposure Period: 28 days

Result : Test material was not readily biodegradable. Half-life was reached by day 25. By day 28, 58.1% degradation of the test material was observed. 10% biodegradation was achieved on day 7.

By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

	% Degradation*	Mean % Degradation

Sample	(day 28)	(day 28)
Test Material	60.1, 60.7, 53.7	58.1
Na Benzoate	87.1, 85.4	86.2

* replicate data

Test condition : Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 57 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Test substance is considered not readily biodegradable.
Reliability : (1) valid without restriction
06.04.2006 (10)

Type : aerobic
Inoculum : activated sludge, domestic
Contact time :
Degradation : = 59.6 (±) % after 28 day(s)
Result : other: not readily biodegradable
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1997
GLP : yes
Test substance :

Remark : Test Type: Manometric Respirometry Test
Exposure Period: 28 days
Result : Test material was not readily biodegradable. Half-life was reached by day 21. By day 28, 59.6% degradation of the test material was observed. 10% biodegradation was achieved on day 8.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	56.5, 60.3, 61.8	59.6
Na Benzoate	92.5, 92.7	92.6

* replicate data

Test condition : Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 50mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Test substance is considered not readily biodegradable.
Reliability : (1) valid without restriction
06.04.2006 (6)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF : 30 - 60
Elimination :
Method : OECD Guide-line 305
Year : 1999
GLP : yes
Test substance :

Remark :

No difference in mortality or growth was observed between the treatments and the control after 10 days of exposure, or at the end of the study (14 days).

The BCF as a function of lipid content was 1087 L/kg and 493.4 L/kg, respectively. The mean BCF as a function of lipid content was 790.2 L/kg.
Duration of test: 10 days uptake, 4 days depuration

The duration of the uptake phase was shorter than the guideline recommended duration of 28 days. The duration of the uptake phase was determined based on the concentration of the test substance reaching a steady state in the tissue of the fish. Samples of the fish were analyzed at regular intervals. To determine the concentration of the test substance in the fish tissue, under steady-state conditions, one-tail T-tests for the comparison of the means at the sampling times were performed.

Result : Calculated Bioconcentration Factor (BCF):
0.16 mg/L = 60
0.04 mg/L = 30
Mean BCF for the study = 45

Test condition : A 100 mg/L stock solution was prepared by adding the appropriate amount of the test substance to 40 liters of dilution water. The stock solution was mixed for 24 hours prior to its use in the test. It was then pumped from the mixing vessel via a glass tube, silicon tubing and varistaltic pump and delivered to the test chambers via a 2 liter proportional diluter. Two concentrations were prepared for the test, 0.16 mg/L and 0.04 mg/L. A dilution water control was also prepared. A new stock solution was prepared in this manner every 3 days and mixed for 24 hours prior to use in the test.
One test chamber was prepared for each treatment and the control. At the start of the test each test chamber contained 45 fish. Fish were observed daily for mortality and/or abnormal behavior or appearance. Water and fish samples were removed periodically during both the uptake and depuration

phases of the study. Samples were analyzed by gas chromatography.
Mean measured concentrations of the test substance in water :
0.16 mg/L = 0.11 mg/L (s.d.= 0.034)
0.04 mg/L = 0.02 mg/L (s.d.= 0.007)
The test substance was not detected in the control during the study or in either treatment during the depuration phase.
Mean measured concentrations of the test substance in fish tissue:
0.16 mg/L = 6.6 mg/kg
0.04 mg/L = 0.60 mg/kg
Fish samples were also removed at the beginning and end of the uptake phase and analyzed for lipid content. The mean percent lipid content was 5.84%.

Test temperature was 14.1 Deg C., Lighting was 16 hours light : 8 hours dark with 545 to 727 Lux during full daylight periods.

Dissolved Oxygen ranged from 9.1 to 9.9 mg/L. The pH was ranged from 7.0 to 7.5 during the study. Fish were fed at a rate of 2% of their bodyweight per day during the study.

Fish Mean Weight was approximately = 0.230g at te start of the test. Test Loading = 0.30 g of fish/L.

The following data represent the measurements of the test chemical in fish tissue. Units are in µg of test chemical per gram of fish. The Non Detect (ND) level was 0.27 µg/g, which corresponds to 0.65 µg/g for a 0.4 g fish mass. All samples taken on Day 4 of the depuration phase resulted in non-detects.

Fish Tissue Analysis

	Uptake Phase			
	Day 1	Day 2	Day 4	Day 10
Control	ND	ND	ND	ND
	ND	ND	ND	ND
0.04mg/l	0.34	0.45	0.52	0.71
	0.56	0.95	0.66	0.79
			0.50	
mean	0.45	0.70	0.59	0.67
0.16mg/l	3.9	4.5	3.7	8.0
	4.2	3.9	3.1	4.5
	6.4	8.2	4.0	9.3
	4.7	7.2	4.5	6.6
mean	4.8	6.0	3.8	7.1

	Depuration Phase				
	Day 0	Day 0	Day 0	Day 1	Day 2
Control	ND	ND	ND	ND	ND
	ND	ND	ND	ND	ND
	ND	ND			
0.04mg/l	0.47	0.40	0.32	ND	ND
	0.46	0.44	0.21	0.33	ND
	0.79	0.42			
	0.67	0.39			
mean	0.60	0.41	0.27	<0.33	ND
0.16mg/l	2.6	2.5	1.9	0.65	0.71
	2.7	2.0	1.0	0.44	0.43
	2.1	2.9	2.3	0.89	

		2.8	2.8	1.7		
	mean	2.6	2.6	1.7	0.66	0.57

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Low potential to bioaccumulate. Value based on wet weight data.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
16.03.2006 (11)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .42 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1998
GLP	:	yes
Test substance	:	

Method : Spearman-Karber Method (Hamilton, et al, 1977)

Result : LC50 = 0.42 mg/L (CI 0.37 to 0.48), based upon measured concentrations of mean of old and new samples.

Analytical method used was GC-MSD

LL50 = 0.64 mg/L (CI 0.57 to 0.73), based upon nominal loading levels.

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
0.25 mg/L	0.17 mg/L	0
0.5 mg/L	0.32 mg/L	13
1.0 mg/L	0.67 mg/L	100
2.0 mg/L	0.94 mg/L	100
5.0 mg/L	0.93 mg/L	100

Test condition : Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.

Test temperature was 13.8 Deg C., Lighting was 16 hours light : 8 hours dark with 551 to 736 Lux during full daylight periods.

Dissolved Oxygen at initiation ranged from 8.3 to 9.2 mg/L and from 6.6 to 8.8 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.6 to 8.2 during the study. Fish were not fed during the study.

Fish Mean Wt.= 0.131g. Mean Total length = 2.7cm, Test Loading = 0.15 g of fish/L.

Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Test substance is considered to have high acute toxicity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (8)

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 1.2 measured/nominal

Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1997
GLP	:	yes
Test substance	:	
Method	:	Probit procedure of SAS (Finney, 1971)
Result	:	LC50 = 1.2 mg/L (CI 0.98 to 1.4), based upon measured concentrations of mean of old and new samples. Analytical method used was GC-MSD LL50 = 1.7 mg/L (CI 1.4 to 3.3), based upon nominal loading levels.

Nominal Conc.	Measured Conc.	% Mortality @ 96 hr.
Control	Below detection	0
0.4 mg/L	0.22 mg/L	0
0.75 mg/L	0.43 mg/L	7
1.5 mg/L	1.13 mg/L	33
3.0 mg/L	1.18 mg/L	100
6.0 mg/L	1.78 mg/L	100

		Dissolved oxygen levels dropped below 60% (40-60%) of saturation in some of the treatments on Days 1 through 4 of the test. Based on mortality observations, these deviations are not believed to have affected the outcome of the study.
Test condition	:	Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution. Test temperature was 15.1 Deg C., Lighting was 16 hours light : 8 hours dark with 749 to 752 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.5 to 9.8 mg/L and from 3.9 to 8.0 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.6 to 8.1 during the study. Fish were not fed during the study. Fish Mean Wt.= 0.623g. Mean Total length = 4.3cm, Test Loading = 0.69 g of fish/L.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Test substance is considered to have moderate acute toxicity.
Reliability	:	(1) valid without restriction
06.04.2006		(9)

Type	:	
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .15 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR

model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C13 alcohol with a Kow of 5.19.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Based on the calculated Kow value, the C13 alcohol is expected to have an acute 96-hour LC50 of 0.15 mg/L and a Chronic Value of 0.03 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = .71 measured/nominal
Analytical monitoring : yes
Method : EPA OTS 797.1300
Year : 1986
GLP : no data
Test substance :

Method : Probit procedure based on Litchfield-Wilcoxon (1949)
Remark : Test Type: Daphnid Acute Toxicity Test
Result : 48-hour LC50 = 0.71 mg/L (CI 0.59 - 0.85) as Total Carbon, based upon mean measured concentrations of Day 0 and Day 2 samples. 48-hour LC50 value equivalent to 16.7% WSF.

Analytical method used was Total Carbon

Nominal Conc.	Measured Conc.	% Mortality @ 48 hr.
Control	-	0
6.25% WSF	0.28 mg/L	0
12.5% WSF	0.58 mg/L	30
25% WSF	1.03 mg/L	85
50% WSF	1.85 mg/L	100
100% WSF	4.17 mg/L	100

Test condition : The water soluble fraction (WSF) was prepared by combining the test substance with dilution water at a ratio of 1:150. The solutions were mixed for 96 hours and allowed to settle for 1 hour prior to use as the 100% WSF stock solution. Test solutions were prepared by diluting the 100% WSF stock. Two replicates of 250 mL in 400 mL autoclaved glass beakers were prepared at each treatment level. Ten daphnids per replicate chamber. Test chambers were covered with glass and placed in a temperature-controlled waterbath. The test was performed under static conditions.

Test temperature was 20.8 Deg C., Lighting was 16 hours light : 8 hours

dark with 57.5 to 67.3 footcandles during full daylight periods. Dissolved oxygen ranged from 8.1 to 9.1 mg/L during the study. The pH was ranged from 7.8 to 8.2 during the study. Dilution water hardness was 130 mg/L as CaCO3.

Organisms were supplied by in-house cultures. Age = <24 hours old from 19-day old parents.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Test substance is considered to have high acute toxicity.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
06.04.2006 (4)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
EC50 : = .81 measured/nominal
Analytical monitoring : yes
Method : OECD Guide-line 202
Year : 1997
GLP : yes
Test substance :

Method : Probit procedure of SAS (Finney, 1971)
Remark : Test Type: Daphnid Acute Toxicity Test
Result : 24-hour EC50 = 0.81 mg/L (Could not calculate CI), based upon measured concentrations of mean of old and new samples.

Analytical method used was GC-MSD

Nominal Conc.	Measured Conc.	% Immobilization @ 24 hr.
Control	Below detection	0
0.31 mg/L	0.45 mg/L	25
0.63 mg/L	1.14 mg/L	85
1.25 mg/L	1.75 mg/L	100
2.5 mg/L	2.3 mg/L	95
5.0 mg/L	2.5 mg/L	100

Test condition : Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 2.0L of dilution water in a 2L glass aspirator bottle. The solutions were mixed for 23 hours at a vortex of </= 10% of the total depth. The test solutions were removed through the outlet at the bottom of each mixing vessel into four replicates of 140 mL in 125 mL glass erlenmeyer flasks (no headspace). Five daphnids were added to each test replicate and the replicates sealed. The test was performed under static conditions with no aeration.

Test temperature was 19.8 Deg C., Lighting was 16 hours light : 8 hours dark with 443 to 577 Lux during full daylight periods. Dissolved oxygen ranged from 8.0 to 8.5 mg/L during the study. The pH was ranged from 7.0 to 7.6 during the study.

Organisms were supplied by in-house cultures. Age = <24 hours old.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : The results of this study confirm the EC50 is below 1.0 mg/L.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
06.04.2006 (5)

Type :
Species : Daphnia sp. (Crustacea)

Exposure period	:	48 hour(s)
Unit	:	mg/l
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C13 alcohol with a Kow of 5.19.

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Based on the calculated Kow value, the C13 alcohol is expected to have an acute 48-hour EC50 of 0.2 mg/L and a Chronic Value of 0.04 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

06.04.2006 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: Pseudokirchneriella subcapitata
Endpoint	:	
Exposure period	:	72 hour(s)
Unit	:	mg/l
EC50	:	= 2.6 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	2003
GLP	:	yes
Test substance	:	

Method : Statistical methods-EC50 was determined using Maximum likelihood analysis based on D.J. Finney (1971). NOECs were determined using the ANOVA procedure of SAS.

Result : 72 hour EC50b = 2.6mg/L (biomass)
72 hour EC50gr = 3.2mg/L (growth rate)
72 hour NOECRb = 1.5mg/L (biomass)
72 hour NOECRgr = 2.2mg/L (growth rate)

Analytical method used was GC-FID.

Nominal Conc. (mg/L)	Mean Cell Growth - 72 hr (% Inhibition)	Conc. - 72 hr (cells/ml)
Control	n/a	8.3 x10E5
1.5 (1.5)*	3.1	7.9 x10E5

3.0 (2.2)	7.2	7.7 x10E5
8.0 (2.2)	21	7.6 x10E5
20 (2.5)	49	4.7 x10E5
61 (3.0)	86	1.1 x10E5

*note - value in parentheses is mean measured concentration (mg/L)
n/a - Not applicable

Test condition : Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 2L of dilution water in a 2L glass bottle. The solution was mixed for 23 hours at a vortex of 8% of the total depth. Mixing temperature was approximately 23 Deg C. After a 1-hour settling/cooling period, the aqueous portions were transferred to the test chambers via the port at the bottom of the mixing vessel and used for testing. Test vessels were 125ml glass Erlenmeyer flasks that were filled with approximately 60ml of treatment solution and inoculated with algae. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1.0 x 104 cells/ml. All test replicates were placed on a shaker table at 100 oscillations per minute during the study. Biomass was calculated as the area under the growth curve.

Test temperature was 23.1 Deg. C. Lighting was continuous at 7600 to 7800 Lux. The pH ranged from 7.3 to 7.4 at test initiation and ranged from 6.8 to 7.1 at termination.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Test substance is considered to have moderate to high acute toxicity to algae.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.04.2006 (13)

Species : other algae: green alga
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = .15 calculated
Method : other: ECOSAR Computer Model
Year : 2005
GLP :
Test substance :

Test condition : Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using a C13 alcohol with a Kow of 5.19.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion : Based on the calculated Kow value, the C13 alcohol is expected to have an acute 96-hour EC50 of 0.15 mg/L and a Chronic Value of 0.09 mg/L.
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
06.04.2006 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= .03 calculated
Method	:	other: calculated
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C13 alcohol with a Kow of 5.19.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Based on the calculated Kow value, the C13 alcohol is expected to have a 30-day Chronic Value of 0.03 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by ECOSAR. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia sp. (Crustacea)
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= .04 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C13 alcohol with a Kow of 5.19.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Based on the calculated Kow value, the C13 alcohol is expected yo have a 16-day EC50 of 0.04 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: Earthworm
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/kg soil dw
LC50	:	= 128.32 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2005
GLP	:	
Test substance	:	
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate acute terrestrial toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard, which is a subroutine in the EPIWIN computer model. KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using a C13 alcohol with a Kow of 5.19.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Based on the calculated Kow value, the C13 alcohol is expected to have a 14-day EC50 of 128.32 mg/kg soil.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (3)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: None
Doses	:	2000 mg/kg bw
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1988
GLP	:	yes
Test substance	:	
Remark	:	Route of administration: Oral Gavage Frequency of Treatment: Single Dose Dose/Concentration Levels: 2000 mg/kg Control group and Treatment: None There were no deaths in males or females. Clinical signs of toxicity that were observed included sedation, diarrhea and dyspnea (males). There were no macroscopic changes observed at necropsy.
Result	:	LD50 > 2000 mg/kg
Test condition	:	The testing procedure used in this study is in accordance with OECD Guidelines 401. After being fasted for 12 to 18 hours, male and female rats were administered a single oral gavage dose of 2,000 mg/kg of the test article. Observations were made four times on day 1; and daily for 14 days. Animals were necropsied at the termination of the study.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Conclusion	:	Under the conditions of this study, Alcohols, C11-14 iso, C13 rich has a low order of acute oral toxicity in rats.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (26)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other: IRT
Value	:	> 12 ppm
Species	:	rat
Strain	:	Wistar
Sex	:	
Number of animals	:	10
Vehicle	:	other: none
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other
Year	:	
GLP	:	no
Test substance	:	
Remark	:	Observations were made for mortality, signs of toxic effect, and body wight changes during a 24-hour post-exposure observation period. Feed and water were freely available during the post-exposure holding period.

Nearly saturated atmospheres were generated by fritted-disk bubblers containing a measured amount of the test substance through which all air entering the chambers was passed. Chamber concentrations were not determined. The nominal concentration was determined by the net loss of the test substance from the bubblers and the total airflow.

Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Reliability : (2) valid with restrictions
Pre-GLP from peer reviewed literature.
Flag : Critical study for SIDS endpoint
06.04.2006 (30)

Type : other: IRT
Value : > 12 ppm
Species : mouse
Strain : Swiss
Sex :
Number of animals : 10
Vehicle : other: none
Doses :
Exposure time : 6 hour(s)
Method : other
Year :
GLP : no
Test substance :

Remark : Observations were made for mortality, signs of toxic effect, and body wight changes during a 24-hour post-exposure observation period. Feed and water were freely available during the post-exposure holding period. Nearly saturated atmospheres were generated by fritted-disk bubblers containing a measured amount of the test substance through which all air entering the chambers was passed. Chamber concentrations were not determined. The nominal concentration was determined by the net loss of the test substance from the bubblers and the total airflow.
Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Reliability : (2) valid with restrictions
Pre-GLP from peer reviewed literature.
Flag : Critical study for SIDS endpoint
06.04.2006 (30)

Type : other: IRT
Value : > 12 ppm
Species : guinea pig
Strain : other: English shorthair
Sex :
Number of animals : 10
Vehicle :
Doses :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance :

Remark : Observations were made for mortality, signs of toxic effect, and body wight changes during a 24-hour post-exposure observation period. Feed and water were freely available during the post-exposure holding period. Nearly saturated atmospheres were generated by fritted-disk bubblers containing a measured amount of the test substance through which all air entering the chambers was passed. Chamber concentrations were not determined. The nominal concentration was determined by the net loss of the test substance from the bubblers and the total airflow.
Test substance : CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich

Reliability	:	(2) valid with restrictions Pre-GLP from peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (30)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2600 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	4
Vehicle	:	other: none
Doses	:	0.10, 0.316, 1.00, 3.16 ml/kg
Method	:	OECD Guide-line 402 "Acute dermal Toxicity"
Year	:	1973
GLP	:	no
Test substance	:	
Test condition	:	The test substance was applied volumetrically to the closely clipped, intact abdominal skin at full-strength. The exposed area was covered with an occlusive binding of dental damming for 24-hours. After the exposure, the binding was removed, and the remaining material, if any, was cleaned from the skin. Water and feed was freely available to the animals and no mechanical restraints were used. Observations for signs of toxicity were made frequently on the day of application and once daily afterward for a total of 7 days. Observations for dermal irritation were made on a daily basis. Gross necropsies were performed at the end of the experiment.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Reliability	:	(2) valid with restrictions Pre-GLP from peer reviewed literature.
Flag	:	Critical study for SIDS endpoint

06.04.2006 (30)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	.5 undiluted
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	
PDII	:	2.4
Result	:	moderately irritating
Classification	:	
Method	:	other: OECD TG 404; EEC Directive 84/449, section B4
Year	:	1989
GLP	:	yes
Test substance	:	
Remark	:	Mean scores at 24, 48, and 72 hours were 2.0, 2.0, and 2.0 for erythema and 0.33, 0 and 0 for edema, respectively.

		Three male and three female (14 to 15 weeks old) New Zealnd White rabbits were used.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. Approximately 24 hours prior to application of the test substance, the dorsal fur was shaved with an electric clipper. On Day 1 of the study, 0.5 ml of the test substance was applied to the skin of the animal and covered with a 3.0 cm x 3.0cm patch of surgical gauze, which was then covered by a semi-occlusive dressing. The dressing was removed four hours after the application and the skin was flushed with lukewarm water. The skin reaction was assessed according to the test guidelines at 1, 24, 48, and 72 hours and at 7 days after the removal of the dressing.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (28)

Species	:	rabbit
Concentration	:	.5 undiluted
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	
PDII	:	1.8
Result	:	slightly irritating
Classification	:	not irritating
Method	:	other: OECD TG 404; EEC Directive 84/449, section B4
Year	:	1993
GLP	:	yes
Test substance	:	

Remark	:	Male and female New Zealand White rabbits (12 to 16 weeks old) were used. Mean scores at 24, 48, and 72 hours were 1.33, 1.0, and 1.0 for erythema and 1.17, 0.5 and 0.17 for edema, respectively.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. Approximately 24 hours prior to application of the test substance, the dorsal fur was shaved with an electric clipper. On Day 1 of the study, 0.5 ml of the test substance was applied to the skin of the animal and covered with a 2.5 cm x 2.5cm patch of surgical gauze, which was then covered by a semi-occlusive dressing. The dressing was removed four hours after the application and any residual test substance was removed by gently swabbing with cotton wool soaked in diethyl ether. The skin reaction was assessed according to the Draize Method at 1, 24, 48, and 72 hours and at 7 days after the removal of the dressing.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (29)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	.1 undiluted
Dose	:	
Exposure time	:	
Comment	:	

Number of animals	:	6
Vehicle	:	
Result	:	moderately irritating
Classification	:	
Method	:	other: OECD TG 405; EEC 84/449, section B.5
Year	:	1988
GLP	:	yes
Test substance	:	
Remark	:	Mean scores at 24, 48, and 72 hours were 1.7, 1.3, 0.7 for conjunctival redness, 0.7, 0.3, 0 for chemosis, 0, 0.7, 0.3 for iridial irritation, and 1.0, 1.0 and 1.0 for corneal opacity, respectively. No staining of the cornea and conjunctivae was observed in the rabbits during the entire test period which could be related to test article effects. No corrosion effect was observed at each measuring interval. No acute toxicological signs were observed in the animals during the test period. Three male and three female New Zealand White rabbits (14 to 15 weeks old) were administered a single instillation.
Test condition	:	Animals were individually housed in stainless steel cages, with adequate food and water. The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together for approximately 1 second to prevent loss of the material. The contralateral eye served as the control. In 3 of the 6 rabbits, approximately 30 seconds after treatment the treated eye was flushed with lukewarm physiological saline for about one minute. The eyes of each animal were examined 1, 24, 48, and 72 hours, and 7 and 14 days after administration. At each interval the treated and control eyes were examined and scored for ocular reactions according to the Draize Standard Eye Irritation Grading Scale. Body weights were recorded on Day 1 and at termination of the test.
Test substance	:	CAS No. 68526-86-3; alcohols, C11-14-iso, C13 rich
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2006 (27)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	14 days
Frequency of treatm.	:	permanent by diet
Post exposure period	:	
Doses	:	0, 100, 500, 2000 mg/kg bw/day
Control group	:	yes
NOAEL	:	= 2000 mg/kg bw
NOEL F1	:	= 2000 mg/kg bw

Method	:	other: Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
Year	:	
GLP	:	yes
Test substance	:	other TS: Analog substance 1-dodecanol (CAS No. 112-53-8)
Remark	:	Test Types: One generation study Premating exposure period: 14 days for both male and female
Result	:	No effects were seen on reproductive or developmental parameters up to doses of 2000 mg/kg bw/day. 1-Dodecanol in the doses administered had no influence on body weight, weight gain, food consumption and food efficiency in the parental generation. Pregnancy rates were not statistically altered and there were no differences in the lengths of the gestation periods. No organ toxicity was observed in the females. There was no effect on the number of pups per litter, weight, sex ratio or mortality rate from days 1-5 after birth. Autopsy indicated no effect from 1-Dodecanol under the conditions of this experiment.
Test substance	:	1-dodecanol (CAS No. 112-53-8) 99% Dodecanol from Sigma (# L 5375) was tested.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

06.04.2006 (18)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	S. typhimurium, E. coli
Test concentration	:	0.01, 0.05, 0.1, 0.5, 1, 5, 10, and 50 ug/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other
Year	:	1985
GLP	:	no data
Test substance	:	
Method	:	Samples run in duplicate. No further details provided.
Remark	:	Strain: Salmonella typhimurium /TA98; TA100; TA1535; TA1537; TA1538; E. coli WP2uvrA
Result	:	There was no evidence of mutagenicity of 1-dodecanol in the presence or absence of metabolic activation in all of the strains tested. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 1-dodecanol samples.
Test condition	:	1-dodecanol (90% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls.
Test substance	:	Analog Substance: 1-Dodecanol (CAS No. 112-53-8)
Conclusion	:	1-Dodecanol was not mutagenic in bacteria under the conditions of this study.
Reliability	:	(2) valid with restrictions (Similar to OECD 471)
Flag	:	Critical study for SIDS endpoint

06.04.2006 (31)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	other: albino mice, CFW 1
Route of admin.	:	gavage
Exposure period	:	24, 48, and 72 hours
Doses	:	5000 mg/kg body weight
Result	:	negative
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	1989
GLP	:	yes
Test substance	:	
Result	:	No statistically significant enhanced mean values of micronucleated cells in polychromatic erythrocytes were seen following oral doses of 5000 mg/kg body weight. No reduction in the ratio of polychromatic to normochromatic erythrocytes was seen.
Test substance	:	Analog substance: 1-dodecanol (CAS. 112-53-8)
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

06.04.2006 (2)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral feed
Exposure period	:	14 days
Frequency of treatm.	:	permanent by diet
Duration of test	:	5 weeks
Doses	:	0, 100, 500, 2000 mg/kg bw/day
Control group	:	yes
NOAEL maternal tox.	:	= 2000 mg/kg bw
NOAEL teratogen.	:	= 2000 mg/kg bw
other: NOEL F1 Offspring	:	= 2000 - mg/kg bw
Method	:	other: Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
Year	:	
GLP	:	yes
Test substance	:	
Remark	:	Test Type: One generation study Premating exposure period: 14 days for both male and female
Result	:	No effects were seen on reproductive or developmental parameters up to doses of 2000 mg/kg bw/day. 1-Dodecanol in the doses administered had

no influence on body weight, weight gain, food consumption and food efficiency in the parental generation. Pregnancy rates were not statistically altered and there were no differences in the lengths of the gestation periods. No organ toxicity was observed in the females. There was no effect on the number of pups per litter, weight, sex ratio or mortality rate from days 1-5 after birth. Autopsy indicated no effect from 1-Dodecanol under the conditions of this experiment.

Test substance : Analog substance: 1-dodecanol (CAS. 112-53-8)
99% Dodecanol from Sigma (# L 5375) was tested.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

06.04.2006 (17)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT